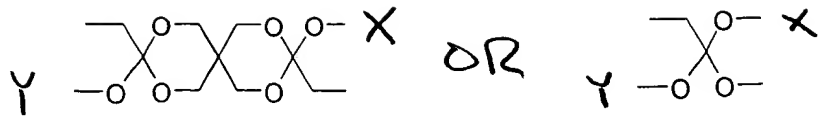
STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 107837

TO: Richard Schnizer Location: CM1/12E17/11E12 Art Unit : 1635 Friday, November 07, 2003 Case Serial Number: 09778388	From : Susan Hanley Location: Biotech-Chem Library CM1 6B05 Phone: 305-4053 susan.hanley@uspto.gov

Search Notes

Compounds =



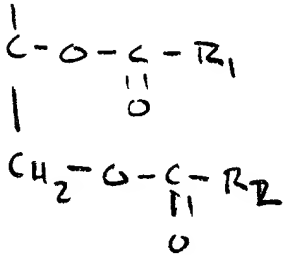
WHERE

Y = anything

X = straight or branched chain alkyl, alkoxy, or acyl, saturated or unsaturated

OR

X =

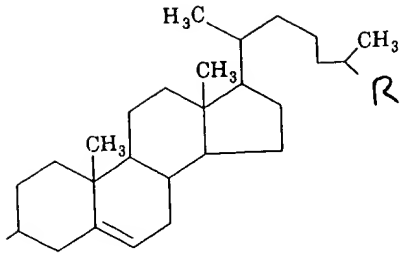


R_1 and R_2 are independent C_1-C_{30} alkyl saturated or unsaturated

OR

(Cont'd next page)

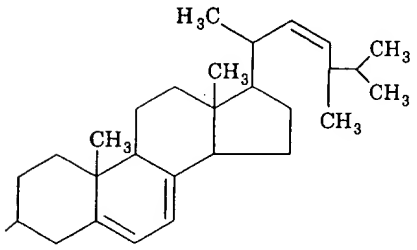
X=



R= C_2H_5, or CH_3

OR

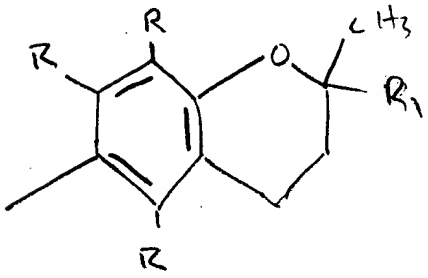
X=



Ergosterol

OR

X=



R = H or CH_3

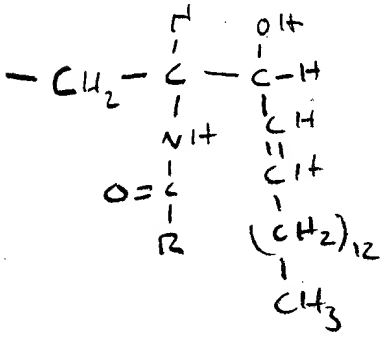
$R_1 = (CH_2CH_2CH_2\underset{\displaystyle CH_3}{\underset{|}{C}}H)_3-CH_3$

OR

$(CH_2CH_2CH=\underset{\displaystyle CH_3}{\underset{|}{C}})_2-CH_3$

OR

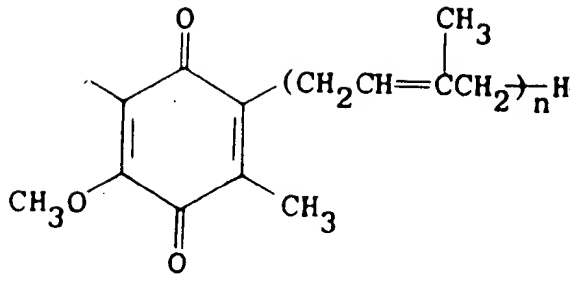
X=



R = C_1-C_{20} alkyl, saturated or unsaturated.

OR (cont'd next page)

X=



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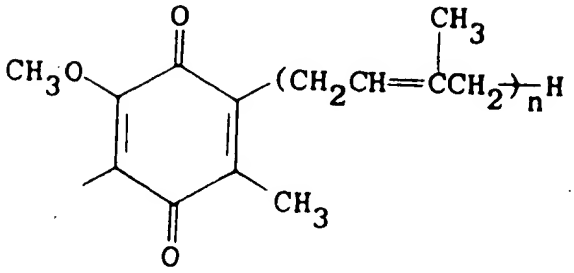

If there are too many hits, please try to search with Y= polyethyleneglycol, hydroxylated dendrons, poly(methyloxazoline), poly(ethyloxazoline), or polyvinylpyrrolidone.

Please also search hit lists with the terms (liposom? or emulsion or micell? or lipid?.)
(I need results with and without this set of terms)

cpds related to suggested terms

SCHNIZER 09/778,388

packet #1

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=> d que l28
L20                STR
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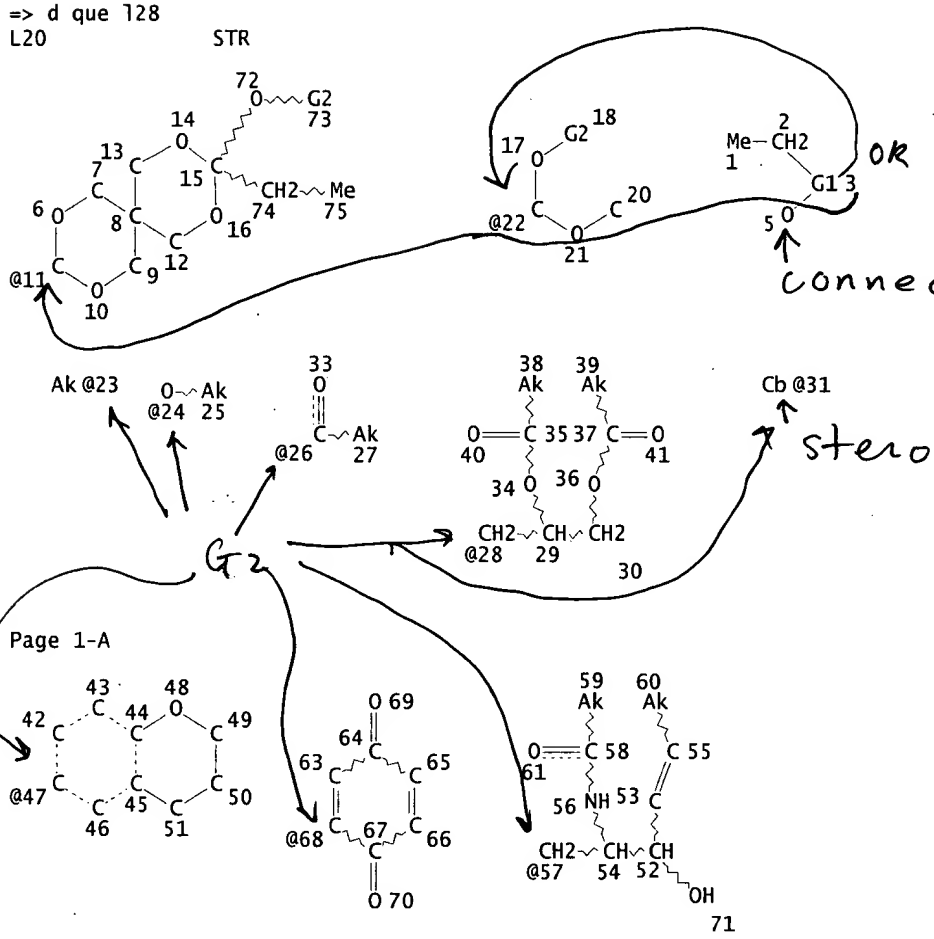

Page 1-A

Page 2-A
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CONNECT IS E1 RC AT 25
CONNECT IS E1 RC AT 27
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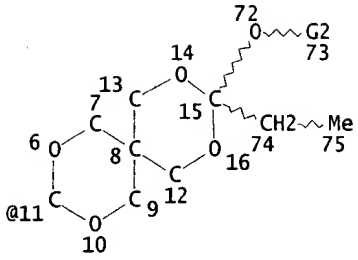
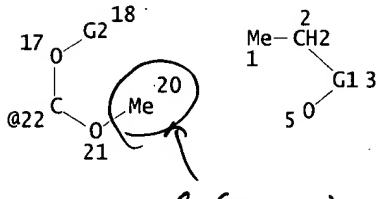
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY UNS AT 31
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E17 C AT 31

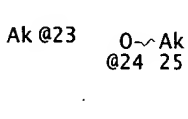
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 71

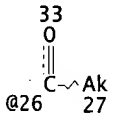
STEREO ATTRIBUTES: NONE
L23 50 SEA FILE=REGISTRY SSS FUL L20 50 cpds from full STR search
L24 STR subset STR

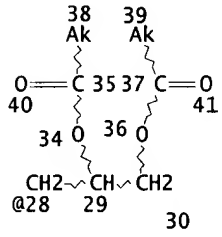




C (open) to methyl







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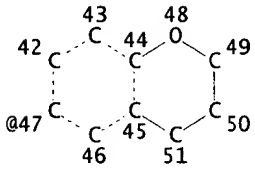
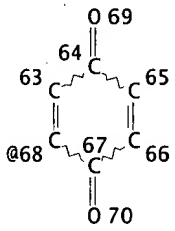
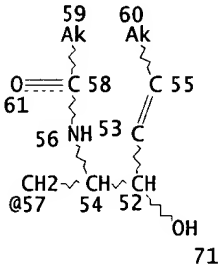
Page 1-A







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DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E17 C AT 31

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 71

STEREO ATTRIBUTES: NONE
L25 13 SEA FILE=REGISTRY SUB=L23 SSS FUL L24 13 cpds
L26 67 SEA FILE=CAPLUS ABB=ON PLU=ON L25 67 refs
L28 4 SEA FILE=CAPLUS ABB=ON PLU=ON L26 AND (LIPOSOM? OR LIPID? OR MICELL? OR EMULSION) 4 cites

=> d ibib abs hitstr l28 1
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

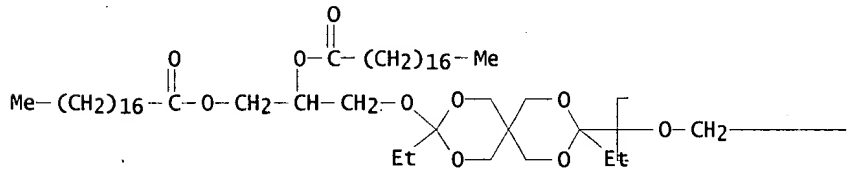
L28 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:223217 CAPLUS
DOCUMENT NUMBER: 139:2656
TITLE: Mechanism of pH-triggered collapse of phosphatidylethanolamine **liposomes** stabilized by an ortho ester polyethyleneglycol **lipid**
AUTHOR(S): Guo, Xin; MacKay, J. Andrew; Szoka, Francis C., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, University of California at San Francisco, San Francisco, CA, 94143-0446, USA
SOURCE: Biophysical Journal (2003), 84(3), 1784-1795
CODEN: BIOJAU; ISSN: 0006-3495
PUBLISHER: Biophysical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

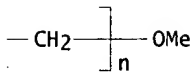
AB The mechanism of pH-triggered destabilization of **liposomes** composed of a polyethyleneglycol-orthoester-distearoylglycerol **lipid** (POD) and phosphatidyl ethanolamine (PE) has been studied using an ANTS/DPX leakage and a **lipid**-mixing assay. We developed a kinetic model that relates POD hydrolysis to **liposome** collapse. This min.-surface-shielding model describes the kinetics of the pH-triggered release of POD/PE **liposomes**. In the model, when acid-catalyzed hydrolysis lowers the mole percentage of POD on the **liposome** surface to a crit. level, intervesicular **lipid** mixing is initiated, resulting in a burst of contents release. Two phases of content leakage are obsd.: a lag phase and a burst phase. During the lag phase, less than 20% of **liposomal** contents are released and the leakage begins to accelerate when approaching to the transition point. During the burst phase, the leakage rate is dependent on interbilayer contact. The burst phase occurs when the surface d. of the PEG **lipid** is 2.3.+-.0.6 mol%, regardless of the pH. Vesicles contg. 4 mol% of a pH-insensitive PEG-**lipid** conjugate and 10% POD did not leak contents or collapse at any pH. These data are consistent with the stalk theory to describe the lamellar-to-inverted hexagonal phase transition and set a lower bound of .apprx.16 PE **lipids** on the external monolayer as the contact site required for **lipid** mixing between two bilayers.

IT **335105-03-8**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(mechanism of pH-triggered collapse of phosphatidylethanolamine **liposomes** stabilized by an ortho ester polyethyleneglycol **lipid**)

RN 335105-03-8 CAPLUS
CN Poly(oxy-1,2-ethanediyl), .alpha.-[9-[2,3-bis[(1-oxooctadecyl)oxy]propoxy]-3,9-diethyl-2,4,8,10-tetraoxaspiro[5.5]undec-3-yl]-.omega.-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A





REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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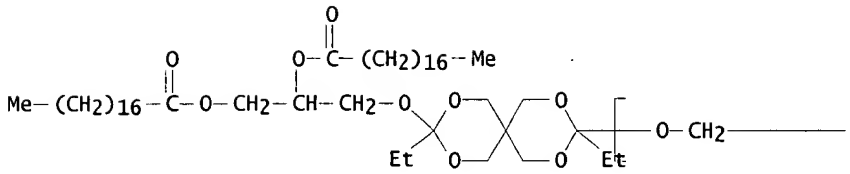
L28 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:98129 CAPLUS
DOCUMENT NUMBER: 138:292609
TITLE: Low-pH-Sensitive PEG-Stabilized Plasmid-**Lipid** Nanoparticles: Preparation and Characterization
AUTHOR(S): Choi, Joon Sig; MacKay, J. Andrew; Szoka, Francis C., Jr.
CORPORATE SOURCE: Department of Biopharmaceutical Sciences and Pharmaceutical Chemistry, University of California at San Francisco, San Francisco, CA, 94143-0446, USA
SOURCE: Bioconjugate Chemistry (2003), 14(2), 420-429
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The acid-labile poly(ethylene glycol) diorthoester distearoylglycerol **lipid** (POD) was used with a cationic **lipid** -phosphatidylethanolamine mixt. to prep. stabilized plasmid-**lipid** nanoparticles (POD SPLP) that could mediate gene transfer in vitro by a pH triggered escape from the endosome. Nanoparticles of 60 nm diam. were prepd. at pH 8.5 using a detergent dialysis method. The DNA encapsulation efficiency in the nanoparticles was optimal between 10 and 13 mol % ratio of cationic **lipid** and at a POD content of 20 mol %. The apparent .zeta. potential of the nanoparticles at 1 mM salt and pH 7.5 was pos., indicating cationic **lipid** on the external surface. However, the external layer of the nanoparticles was depleted in the cationic component compared to the starting mole ratio. Low pH sensitivity of the POD SPLP was characterized by a lag phase followed by a rapid collapse; at pH 5.3 the nanoparticles collapsed in 100 min. Nanoparticles prepd. from a pH-insensitive PEG-**lipid**, PEG-distearoylglycerol had similar physicochem. characteristics as the POD SPLP but did not collapse at low pH. The POD SPLP had up to 3 orders of magnitude greater gene transfer activity than did the pH-insensitive nanoparticles. Both the pH-sensitive and pH-insensitive nanoparticles were internalized to a qual. similar extent in a punctate pattern into cultured cells within 2 h of incubation with the cells; thus, increased gene transfer of the POD SPLP was due to a more rapid escape from the endosome rather than to greater cell assocn. of these nanoparticles. These results suggest that the pH-sensitive stabilized plasmid-**lipid** nanoparticles may be a useful component of a synthetic vector for parenterally administered gene therapy.

IT **335105-03-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and characterization of low-pH-sensitive PEG-stabilized plasmid DNA-**lipid** nanoparticles)
RN 335105-03-8 CAPLUS
CN Poly(oxy-1,2-ethanediyl), .alpha.-[9-[2,3-bis[(1-oxooctadecyl)oxy]propoxy]-3,9-diethyl-2,4,8,10-tetraoxaspiro[5.5]undec-3-yl]-.omega.-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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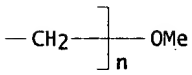

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L28 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:115683 CAPLUS
DOCUMENT NUMBER: 134:315979
TITLE: Steric Stabilization of Fusogenic **Liposomes** by a Low-pH Sensitive PEG-Diortho Ester-**Lipid** Conjugate
AUTHOR(S): Guo, X.; Szoka, F. C., Jr.
CORPORATE SOURCE: Departments of Pharmaceutical Chemistry and Biopharmaceutical Sciences, University of California at San Francisco, San Francisco, CA, 94143-0446, USA
SOURCE: Bioconjugate Chemistry (2001), 12(2), 291-300
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe the synthesis and characterization of a pH-sensitive poly(ethylene glycol)-diortho ester-distearoyl glycerol conjugate (POD). POD was prepd. by a one-step synthesis, and its acid sensitivity characterized by TLC. The conjugate was found to be stable at neutral pH for greater than 3 h but degraded completely within 1 h at pH 5. **Liposomes** composed of 10% of POD and 90% of a fusogenic **lipid**, dioleoyl phosphatidylethanolamine (DOPE) were readily prepd. and remained stable for up to 12 h in neutral buffer as shown by photon correlation spectrometry and a **liposome** contents leakage assay. However, when POD/DOPE **liposomes** were incubated in acidic pH as mild as 5.5, they aggregated and released most of their contents within 30 min. The kinetics of content release from POD/DOPE **liposomes** consisted of two phases, a lag phase, and a burst phase. The lag phase is inversely correlated with pH and the logarithm of the length of lag phase showed a linear relationship with the buffer pH. When the POD/DOPE **liposomes** were incubated in 75% of fetal bovine serum at 37 .degree.C, they remained as stable as traditional PEG-grafted **liposomes** for 12 h but released 84% of the encapsulated ANTS in the following 4 h. Upon i.v. administration into mice, **liposomes** composed of 10% POD and 90% DOPE were cleared from circulation by a one-compartment kinetics with a half-life of about 200 min. POD is an example for the design of a novel category of pH sensitive **lipids** composed of a headgroup, an acid-labile diortho ester linker and a

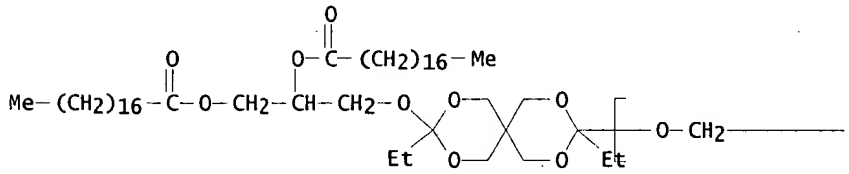
hydrophobic tail. The uniquely fast degrdn. kinetics of POD at pH 5-6 and its ability to stabilize **liposomes** in serum make the conjugate suitable for applications for triggered drug release systems targeted to mildly acidic bio-environments such as endosomes, solid tumors, and inflammatory tissues.

IT **335105-03-8P**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(steric stabilization of fusogenic **liposomes** by a low-pH sensitive PEG-diortho ester-**lipid** conjugate)

RN 335105-03-8 CAPLUS

CN Poly(oxy-1,2-ethanediyl), .alpha.-[9-[2,3-bis[(1-oxooctadecyl)oxy]propoxy]-3,9-diethyl-2,4,8,10-tetraoxaspiro[5.5]undec-3-yl]-.omega.-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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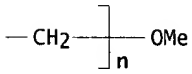

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L28 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1932:14391 CAPLUS
DOCUMENT NUMBER: 26:14391
ORIGINAL REFERENCE NO.: 26:1531a-d
TITLE: Photographic sensitizers
PATENT ASSIGNEE(S): Kodak-Pathe (Soc. anon. francaise)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 712995		19310310	FR	

GI For diagram(s), see printed CA Issue.

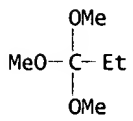
AB Gelatin-Ag halide **emulsions** are sensitized by an 8-alkyl- or 8-arylthiocarbocyanine dye derived from a 2-methyl-.beta.-naphthothiazole. Examples are given of the prepn. of (1) 8-methyl-2,2'-diethyl-3,4,3',4'-dibenzothiocarbocyanine bromide by condensing 2-methyl-.beta.-naphthothiazole with Et p-toluenesulfonate, boiling the product with triethyl orthoacetate in pyridine and adding an excess of NH4Br in hot water; (2) 2,2',8-triethyl-3,4,3',4'-dibenzothiocarbocyanine iodide and (3) 2,2'-dimethyl-8-isoamyl-3,4,3',4'-dibenzothiocarbocyanine iodide. The

general formula of these compds. (A = alkyl or aryl) is: The prepn. of trimethyl orthopropionate used in example (2) is also given. Dry HCl is passed into a chilled mixt. of propionitrile, MeOH and Et2O, and the product is purified. Fr. 713,047, Mar. 11, 1931, describes the prepn. of cyanine dyes for sensitizing **emulsions** from condensation products of .mu.-methylnaphthothiazole. Thus, 1-methyl-.alpha.-naphthothiazole is condensed with Et p-toluenesulfonate, the product is refluxed with Et orthoformate and aq. NH4Br is added to ppt. 2,2'-diethyl-5,6,5',6'-dibenzothiocarbocyanine bromide. The prepn. of 1',2-diethyl-3,4-benzothioisocyanine iodide, 1',2-diethyl-3,4-benzothiopseudocyanine iodide and of others is also given.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester
(prepn. of)

RN 24823-81-2 CAPLUS

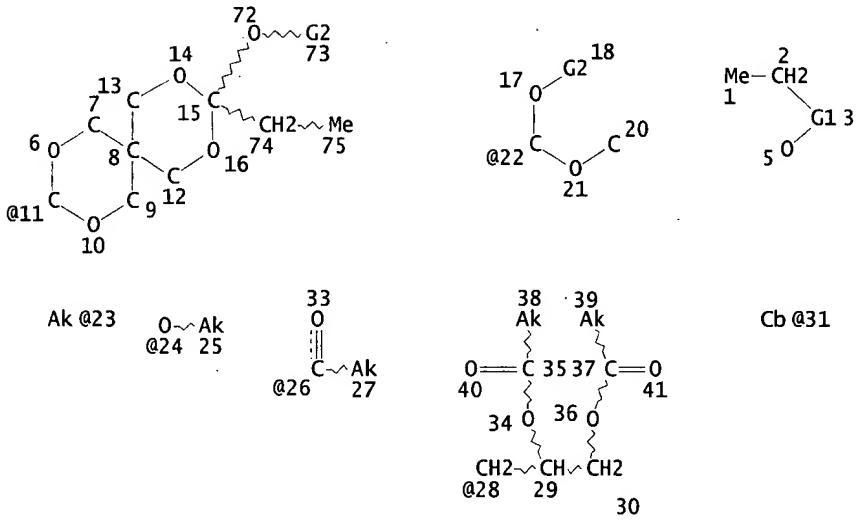
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



same str search as packet #1, (packet #2
these are the remaining references

SCHNIZER 09/778,388

=> d que
L20 STR



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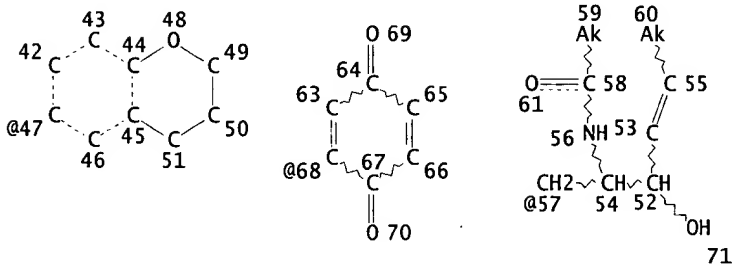

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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 71

STEREO ATTRIBUTES: NONE
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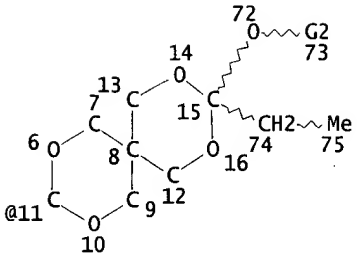
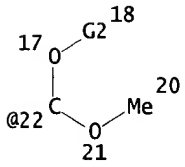
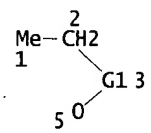
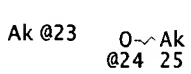
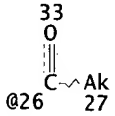
L24 STR

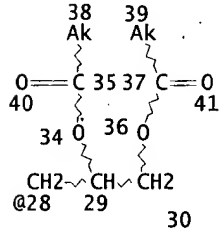












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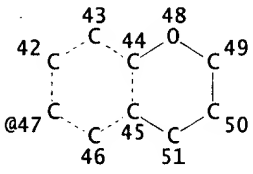

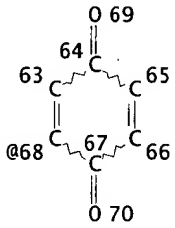

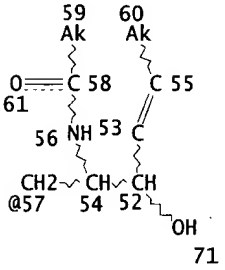

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CONNECT IS E1 RC AT 25
CONNECT IS E1 RC AT 27
CONNECT IS E1 RC AT 38
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 59
CONNECT IS E1 RC AT 60
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY UNS AT 31
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E17 C AT 31

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 71

STEREO ATTRIBUTES: NONE

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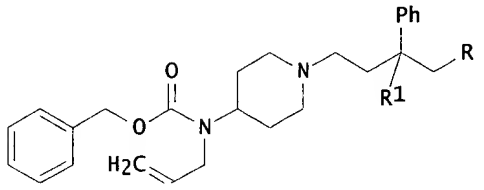
L26	67	SEA FILE=CAPLUS ABB=ON PLU=ON L25
L28	4	SEA FILE=CAPLUS ABB=ON PLU=ON L26 AND (LIPOSOM? OR LIPID? OR MICELL? OR EMULSION)
L29	63	SEA FILE=CAPLUS ABB=ON PLU=ON L26 NOT L28
L30	59	SEA FILE=CAPLUS ABB=ON PLU=ON L29 AND PY<2002

=> d ibib abs hitstr 1-59

L30 ANSWER 1 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:872215 CAPLUS
DOCUMENT NUMBER: 136:325386
TITLE: Design, synthesis, and SAR of heterocycle-containing antagonists of the human CCR5 receptor for the treatment of HIV-1 infection
AUTHOR(S): Kim, Dooseop; Wang, Liping; Caldwell, Charles G.; Chen, Ping; Finke, Paul E.; Oates, Bryan; MacCoss, Malcolm; Mills, Sander G.; Malkowitz, Lorraine; Gould, Sandra L.; DeMartino, Julie A.; Springer, Martin S.; Hazuda, Daria; Miller, Michael; Kessler, Joseph; Danzeisen, Renee; Carver, Gwen; Carella, Anthony; Holmes, Karen; Lineberger, Janet; Schleif, William A.; Emini, Emilio A.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(24), 3103-3106
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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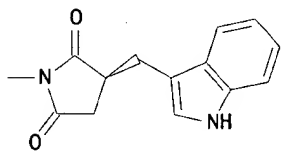
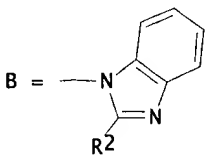
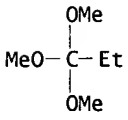
A = 

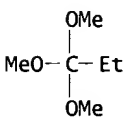
B = 

AB Replacement of the large hydantoin-indole moiety of previously prepd. CCR5 antagonists I (R = Q, R1 = Me, H) with a variety of smaller heterocyclic analogs e.g. I (R = Q1, R1 = Me, H; R2 = H, Et) gave rise to potent CCR5 antagonists having binding affinity comparable to the hydantoin analogs. The synthesis, SAR, and biol. profiles of this class of antagonists are described.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn., anti-HIV and CCR5 receptor antagonist activity, and structure-activity relationship of heterocyclic (benzyloxyamino)piperidines)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



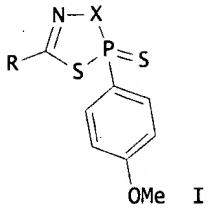
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:557842 CAPLUS
DOCUMENT NUMBER: 133:271512
TITLE: NMR spectral data for ester prodrugs of ganciclovir
AUTHOR(S): Gao, Hongwu; Mitra, Ashim K.
CORPORATE SOURCE: Division of Pharmaceutical Sciences, School of Pharmacy, University of Missouri-Kansas City, Kansas City, MO, 64100-2499, USA
SOURCE: Magnetic Resonance in Chemistry (2000), 38(8), 696-700
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 9-[(1,3-dihydroxy-2-propoxy)methyl]guanine mono- and diesters were synthesized as potential prodrugs of ganciclovir and both 1H NMR and 13C NMR spectra were assigned to these esters based on spectral comparison with compds. of similar structure.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR spectral data for ester prodrugs of ganciclovir)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:306517 CAPLUS
DOCUMENT NUMBER: 132:321921
TITLE: Reaction of the Lawesson reagent with hydrazonates and hydroxamates: synthesis of 1,3,4,2-thiadiazaphospholine sulfides and 1,3,5,2-oxathiazaphospholine sulfides
AUTHOR(S): Boukraa, Mohamed; El Efrit, Mohamed Lotfi; Zantour, Hedi
CORPORATE SOURCE: Laboratoire de Synthese Organique, Departement de Chimie Faculte des Sciences de Tunis, Tunis, Tunisia
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2000), 157, 145-152
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 132:321921
GI



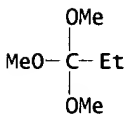
I

AB Lawesson's Reagent ((.mu.-S)2(P(S)C6H4OMe-4)2) reacts with hydrazonates (RC(:NNH2)OMe; R = H, Me, Et, Pr, Ph) and hydroxamates (RC(:NOH)OMe; R = Me, Et, Pr, Ph, PhCH2) to give 1,3,4,2-thiadiazaphospholines (4; shown as I; X = NH) and 1,3,5,2-oxathiazaphospholines (5; shown as I; X = O) derivs. The structures of 4 and 5 were confirmed by IR and NMR spectroscopy.

IT **24823-81-2**, Trimethyl orthopropanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of hydrazonate and/or hydroxamate)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:158953 CAPLUS

DOCUMENT NUMBER: 132:322063

TITLE: Regioselective synthesis of various prodrugs of ganciclovir

AUTHOR(S): Gao, Hongwu; Mitra, Ashim K.

CORPORATE SOURCE: Division of Pharmaceutical Sciences, School of Pharmacy, University of Missouri-Kansas City, Kansas City, MO, 64100-2499, USA

SOURCE: Tetrahedron Letters (**2000**), 41(8), 1131-1136
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

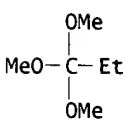
OTHER SOURCE(S): CASREACT 132:322063

AB High-yield regioselective syntheses of 9-[(1,3-dihydroxy-2-propoxy)methyl]guanine mono-, di- and tri-substitution derivs. as potential prodrugs were accomplished via one or multi-steps. Two amino acid esters of ganciclovir were synthesized as water-sol. prodrugs, which form protonated cations in pH 7.4 phosphate buffer.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective synthesis of various prodrugs of ganciclovir)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:811332 CAPLUS
DOCUMENT NUMBER: 132:66473
TITLE: Fuel compositions employing catalyst combustion structure
INVENTOR(S): Orr, William C.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9966009	A2	19991223	WO 1999-US13751	19990617 <--
WO 9966009	A3	20000302		

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2310056	AA	19991223	CA 1999-2310056	19990617 <--
EP 1051461	A2	20001115	EP 1999-928773	19990617 <--

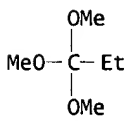
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI

PRIORITY APPLN. INFO.: US 1998-98879 A 19980617
WO 1999-US13751 W 19990617

AB This invention relates to a fuel compn. relating to a broad spectrum of pollution reducing, improved combustion performance, and enhanced stability fuel compns. for use in jet, aviation, turbine, diesel, gasoline, and other combustion applications. More particularly, the present invention relates to metallic vapor phase combustion fuel compns. employing certain co-combustion agents, including trimethoxymethylsilane.

IT **24823-81-2**, 1,1,1-Trimethoxypropane
RL: CAT (Catalyst use); USES (Uses)
(fuel compns. employing catalyst combustion structure)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 6 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:216918 CAPLUS
DOCUMENT NUMBER: 130:252370
TITLE: Preparation of 3-(1,2-benzisothiazol or isoxazolo 5-yl)pyrimidines as herbicides
INVENTOR(S): Wepplo, Peter John; Manfredi, Mark Christopher; Rampulla, Richard Anthony; Cossette, Michael Vernie; Guaciaro, Michael Anthony; Haley, Gregory Jay; Bullock, Billy Gene; Alvarado, Sergio Ivan; Barnes, Keith Douglas; Meier, Gary Allen; Hunt, David Allen;

Carlsen, Marianne; Heffernan, Gavin David
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: PCT Int. Appl., 924 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 9914216	A1	19990325	WO 1998-US19251	19980915	<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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AU 9884239	A1	19990401	AU 1998-84239	19980915	<--
AU 737864	B2	20010830			
AU 9893925	A1	19990405	AU 1998-93925	19980915	<--
ZA 9808435	A	20000315	ZA 1998-8435	19980915	<--
BR 9813017	A	20000815	BR 1998-13017	19980915	<--
JP 2001516758	T2	20011002	JP 2000-511765	19980915	<--
TW 474927	B	20020201	TW 1998-87115446	19980916	
AT 227721	E	20021115	AT 1998-307495	19980916	
ES 2185118	T3	20030416	ES 1998-307495	19980916	
BG 104336	A	20010928	BG 2000-104336	20000413	<--

PRIORITY APPLN. INFO.: US 1997-931451 A 19970917
US 1998-128831 A 19980804
WO 1998-US19251 W 19980915

OTHER SOURCE(S): MARPAT 130:252370
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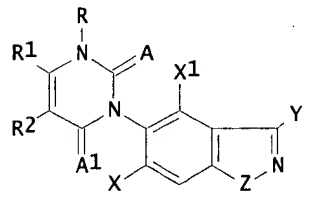

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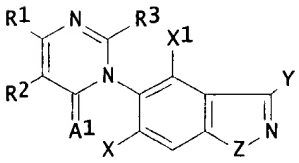


II

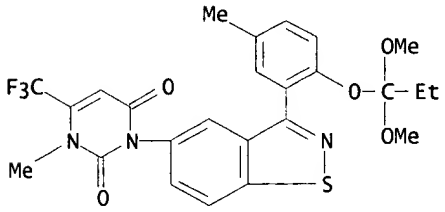
AB Title compds. [I and II; R = alkyl, alkenyl, alkynyl, benzyl; R1 = H, halogen, alkyl, cycloalkyl, alkenyl; R2 = H, halogen, alkyl, cycloalkyl, alkenyl; R3 = halogen; X = H, halogen, alkyl; X1 = H, halogen, alkyl, alkoxy; Z = O, S, SO2, SO; Y = H, halogen, CN, OH, SH, CO2H, CHO, CONH2], optical isomers, diastereomers, and tautomers are prepd. as herbicides in

cereal crop consisting of corn, wheat and rice; further provided are compns. and methods comprising those compds. for the control of undesirable plant species. Thus, title compd. I (R = H; R1 = CF3; R2 = H; A = O; A1 = O; X = H; X1 = H; Y = 3,4-Me2-6-MeOC6H2) were prepd.

IT **221645-52-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-(1,2-benzisothiazol or isoxazolo 5-yl)pyrimidines as herbicides)

RN 221645-52-9 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 3-[3-[2-(1,1-dimethoxypropoxy)-5-methylphenyl]-1,2-benzisothiazol-5-yl]-1-methyl-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:15759 CAPLUS

DOCUMENT NUMBER: 130:124715

TITLE: Calculation of the enthalpies of addition of radicals to aldehydes, ketones, acids, and esters at the C:O bond

AUTHOR(S): Borisov, I. M.; Mikhailov, D. A.; Khursan, S. L.; Yanborisov, V. M.

CORPORATE SOURCE: Bashk. Gos. Univ., Ufa, Russia

SOURCE: Zhurnal Fizicheskoi Khimii (1998), 72(10), 1771-1775
CODEN: ZFKHA9; ISSN: 0044-4537

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

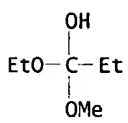
LANGUAGE: Russian

AB Calcns. are presented for the enthalpy of addn. of HO radical to the C and O atoms of the title carbonyl groups, as well as the enthalpy of addn. of MeO, Me, MeOO, and HOO radicals to the C atom of the title carbonyl groups. AM1 dipole moments of the resultant radicals were also reported. The HO radical is predicted to add to the C atom; MeO addn. is weakly exothermic; Me addn. is exothermic with ketones and aldehydes; and peroxyl radicals are unlikely to add to carbonyl groups. Linear .DELTA.H-.mu.(R) correlations (where R represents the radical product of the addn. reaction) were obtained for HO and MeO radicals.

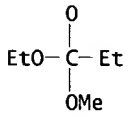
IT **219925-63-0**
RL: PRP (Properties)
(O-H bond energy; calcn. of the enthalpies of addn. of radicals to aldehydes, ketones, acids, and esters at the C:O bond)

RN 219925-63-0 CAPLUS

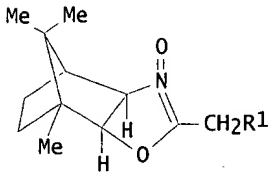
CN 1-Propanol, 1-ethoxy-1-methoxy- (9CI) (CA INDEX NAME)



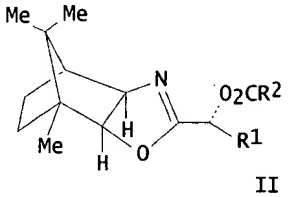
IT **219925-24-3**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation; calcn. of the enthalpies of addn. of radicals to aldehydes, ketones, acids, and esters at the C:O bond)
RN 219925-24-3 CAPLUS
CN Propoxy, 1-ethoxy-1-methoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 8 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:233593 CAPLUS
DOCUMENT NUMBER: 128:308617
TITLE: Stereoselective hetero-Claisen rearrangement of camphor derived oxazoline-N-oxides
AUTHOR(S): Dalko, Peter I.; Langlois, Yves
CORPORATE SOURCE: Laboratoire de Synthese des Substances Naturelles Associe au CNRS, ICMO, Universite de Paris-sud, Orsay, 91405, Fr.
SOURCE: Tetrahedron Letters (**1998**), 39(15), 2107-2110
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:308617
GI

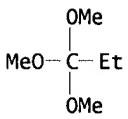


I



II

AB Camphor derived oxazoline-N-oxides I in the presence of various acylating agents afforded .alpha.-acyloxyoxazolines II resulting from a diastereoselective rearrangement. The configuration of the newly formed asym. center was established by chem. correlation. The obsd. diastereoselectivity accounts a concerted rather than a stepwise process.
IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective hetero-Claisen rearrangement of camphor derived oxazoline oxides)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:579788 CAPLUS
DOCUMENT NUMBER: 127:235757
TITLE: Coating composition comprising a bicyclo- or spiro-orthoester-functional compound
INVENTOR(S): Van Den Berg, Keimpe Jan; Hobel, Klaus; Klinkenberg, Huig; Noomen, Arie; Van Oorschot, Josephus Christiaan
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731073	A1	19970828	WO 1997-EP892	19970221 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
NL 1002427	C2	19970826	NL 1996-1002427	19960223 <--
CA 2247126	AA	19970828	CA 1997-2247126	19970221 <--
AU 9720930	A1	19970910	AU 1997-20930	19970221 <--
ZA 9701542	A	19980727	ZA 1997-1542	19970221 <--
EP 882106	A1	19981209	EP 1997-906123	19970221 <--
EP 882106	B1	20000809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1214717	A	19990421	CN 1997-193266	19970221 <--
BR 9707735	A	19990727	BR 1997-7735	19970221 <--
EP 942051	A2	19990915	EP 1999-201141	19970221 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000506908	T2	20000606	JP 1997-529818	19970221 <--
AT 195331	E	20000815	AT 1997-906123	19970221 <--
ES 2150758	T3	20001201	ES 1997-906123	19970221 <--
US 6297329	B1	20011002	US 1997-804485	19970221 <--
RU 2180674	C2	20020320	RU 1998-117558	19970221
TW 418241	B	20010111	TW 1997-86111273	19970806 <--
NO 9803859	A	19981020	NO 1998-3859	19980821 <--
AU 754919	B2	20021128	AU 2000-56513	20000906
US 2002161135	A1	20021031	US 2001-935308	20010822
US 6593479	B2	20030715		

PRIORITY APPLN. INFO.:
NL 1996-1002427 A 19960223
US 1996-15878P P 19960422
EP 1997-906123 A3 19970221
US 1997-804485 A3 19970221
WO 1997-EP892 W 19970221

AB A coating compn. comprises a first compd. of .gtoreq.1 bicyclo- or spiro-orthoester group and a second compd. of .gtoreq.2 hydroxyl-reactive

groups. The latent hydroxyl groups of the bicyclo- or spiro-orthoester groups have to be deblocked and reacted with the hydroxyl-reactive groups of the second compd. to be cured. Bicyclo-orthoester compds. are made from the corresponding oxetane compd., as are polymers comprising .gtoreq.1 bicyclo- or spiro-orthoester group. Thus, Desmodur N 3390 was mixed with 1,4-diethyl-2,6,7-trioxabicyclo[2.2.2]octane in the presence of p-MeC6H4SO3H and Bu2Sn dilaurate in solvent and sprayed onto steel panels showing pot life >1 day and dry time 100 min.

IT **195072-70-9P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(coating compn. comprising a bicyclo- or spiro-orthoester-functional compd. for extended pot life)

RN 195072-70-9 CAPLUS

CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-diethoxy-3,9-diethyl- (9CI) (CA INDEX NAME)

L30 ANSWER 10 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:468421 CAPLUS

DOCUMENT NUMBER: 127:225587

TITLE: Modification of SiO2 surfaces by reaction with acetals, ketals, orthoesters, and orthocarbonates

AUTHOR(S): Guidotti, Bruno R.; Herzog, Erwin; Bangerter, Felix; Caseri, Walter R.; Suter, Ulrich W.

CORPORATE SOURCE: Department Materials, Institute Polymers, ETH, Zurich, CH-8092, Switz.

SOURCE: Journal of Colloid and Interface Science (**1997**), 191(1), 209-215
CODEN: JCISA5; ISSN: 0021-9797

PUBLISHER: Academic

DOCUMENT TYPE: Journal

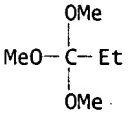
LANGUAGE: English

AB SiO2 was treated with compds. of the type C(OR)4 (orthocarbonates), R'C(OR)3 (orthoesters), and R'R''C(OR)2 (acetals and ketals) in CCl4 under reflux. The modified surfaces were analyzed by IR, 1H NMR, and 13C NMR spectroscopy, and TGA. The initial compds. decomp., leaving on the surface only OR groups that are tightly bound. The reaction with orthocarbonates and orthoesters is more effective than with acetals or ketals, and the SiO2 surface can be covered with OR groups to a high degree. The adsorption of polymers is restricted by the bound org. species. The modified surfaces are similar in many respects to those of alc.-treated silicas, but the reaction proceeds at lower temps. than those typically used for silica modification with alcs.

IT **24823-81-2**, 1,1,1-Trimethoxypropane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(modification of SiO2 surfaces by reaction with)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 11 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:377351 CAPLUS
DOCUMENT NUMBER: 127:18160
TITLE: High-molecular-weight aliphatic polyesters and manufacture method
INVENTOR(S): Kajikawa, Yasuteru; Yamawaki, Kentaro; Matsuda, Akio; Masuda, Takashi
PATENT ASSIGNEE(S): Agency of Industrial Sciences and Technology, Japan; Zaidan Hojin Chikyu Kankyo Sangyo Gijutsu Kenkyusho Kiko
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09095529	A2	19970408	JP 1995-277024	19950929 <--
JP 2700628	B2	19980121		

PRIORITY APPLN. INFO.: JP 1995-277024 19950929

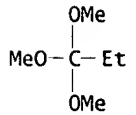
AB The polymers (COR1CO2R2O)kCR3R4(OR2O2CR1CO)p [R1, R2 = divalent aliph. group; R3 = H, aliph. group; R4 = (OR2O2CR1CO)m, OR5; R5 = aliph. or arom. group; , p, m .gtoreq.1; k + p .gtoreq.10; k + p + m .gtoreq.10], having Mn .gtoreq.20,000, good heat resistance, processability, and mech. properties, are prepd. Thus, heating 1,4-butanediol 0.1832, di-Me succinate 0.1765 and tri-Me orthoformate 0.9113 mmol in the presence of Ti(iso-Pr)4 gave a polymer having Mn 51,000, Mw 157,000, and decompn. temp. 305.degree..

IT **189894-44-8P**
RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation) (high-mol.-wt. aliph. polyesters with good heat resistance and processability)

RN 189894-44-8 CAPLUS
CN Butanedioic acid, dimethyl ester, polymer with 1,4-butanediol and 1,1,1-trimethoxypropane (9CI) (CA INDEX NAME)

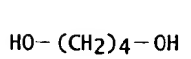
CM 1

CRN 24823-81-2
CMF C6 H14 O3



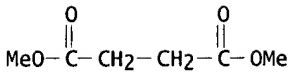
CM 2

CRN 110-63-4
CMF C4 H10 O2

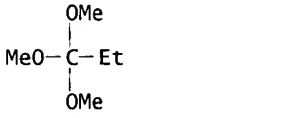


CM 3

CRN 106-65-0
CMF C6 H10 O4



L30 ANSWER 12 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:230976 CAPLUS
DOCUMENT NUMBER: 126:225128
TITLE: Acyclic Stereoselection in the Ortho Ester Claisen Rearrangement
AUTHOR(S): Daub, G. William; Edwards, James P.; Okada, Carol R.; Allen, Jana Westran; Maxey, Claudia Tata; Wells, Matthew S.; Goldstein, Alexandra S.; Dibley, Michael J.; Wang, Clarence J.; Ostercamp, Daniel P.; Chung, Steven; Cunningham, Paula Shanklin; Berliner, Martin A.
CORPORATE SOURCE: Department of Chemistry, Harvey Mudd College, Claremont, CA, 91711, USA
SOURCE: Journal of Organic Chemistry (**1997**), 62(7), 1976-1985
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:225128
AB The ortho ester Claisen rearrangement of trisubstituted allylic alcs. exhibits significant levels of diastereoselection. In E allylic alcs., a 1,3-diaxial interaction develops in the chairlike transition state leading to the anti isomer, rendering the reaction syn selective by a factor of 3-5 to 1. In Z allylic alcs., the 1,3-diaxial interaction develops in the transition state leading to the syn isomer, generating an anti:syn selectivity of 6-15 to 1. The relative stereochem. of the syn isomer was confirmed independently by the synthesis of the mycotoxin botryodiplodin.
IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(acyclic stereoselection in the ortho ester Claisen rearrangement of trisubstituted allylic alcs.)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)

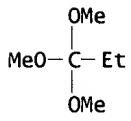


L30 ANSWER 13 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:298443 CAPLUS
DOCUMENT NUMBER: 125:12041
TITLE: Polymer Swelling. Part 18. Sorption of Geminal and Terminal Polyalkoxy-Substituted Alkanes by Poly(styrene-co-divinylbenzene)
AUTHOR(S): Errede, L. A.; Tiers, George V. D.
CORPORATE SOURCE: 3M Corporate Research Laboratories, St. Paul, MN, 55144, USA
SOURCE: Journal of Physical Chemistry (**1996**), 100(23), 9918-9928
CODEN: JPCHAX; ISSN: 0022-3654
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The adsorption parameters (.alpha.) of polyalkoxy alkanes CH4-xZx, CH3-xZx(CH2)nH, and Z(CH2)nCH3-xZx, in which Z is either CH3O or CH3CH2O,

were established exptl. in the usual way. In the cases of those homologous series that comprise the structural classifications CH3-xZx(CH2)nH or Z(CH2)nCH3-xZx, the .alpha.n-values for only 2 or 3 of the lower members (n < 5) in a given series were detd. exptl.; the rest were established by extrapolation or interpolation using the appropriate log .alpha.n vs n linear relationship. The results obtained thereby support the conclusions derived earlier from similar studies in which Z was either a Cl or a Br substituent, namely, that liaison between the adsorbed mol. and the polymer at liq.-satn. is monodentate rather than polydentate. The other Z-substituents on the C atoms adjacent to the adsorption site affect .alpha. in a manner that reflects not only the net influence of electronic and steric contributions at this site but also the affinity of these substituents for the mobile sorbed-but-not-adsorbed mols. in the liq.-satd. system. Hence, systematic incrementation of these Z-substituents to the allowable limit at const. n does not afford a linear log .alpha.x vs x relationship but rather reflects one that exhibits a max. at x = 2 or 3, depending upon the series. On the other hand, similar systematic incrementations of Z on C atoms further removed from the adsorption site do exhibit log .alpha.x vs x linear relationships at const. n in the manner previously noted for log .alpha.n vs n relationships at const. x.

IT **24823-81-2**, 1,1,1-Trimethoxypropane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(sorption of geminal and terminal polyalkoxy-substituted alkanes by poly(styrene-co-divinylbenzene))

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 14 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:994342 CAPLUS
DOCUMENT NUMBER: 124:86709
TITLE: 5-substituted derivatives of mycophenolic acid
INVENTOR(S): Artis, Dean R.; Elworthy, Todd R.; Hawley, Ronald C.; Loughhead, David G.; Morgans, David J., Jr.; Nelson, Peter H.; Patterson, John W., Jr.; Rohloff, John C.; Sjogren, Eric B.; et al.
PATENT ASSIGNEE(S): Syntex (U.S.A.) Inc., USA
SOURCE: PCT Int. Appl., 142 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9522538	A1	19950824	WO 1995-US1787	19950216 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, UG				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5493030	A	19960220	US 1994-198749	19940218 <--
CA 2183530	AA	19950824	CA 1995-2183530	19950216 <--
AU 9518754	A1	19950904	AU 1995-18754	19950216 <--

ZA 9501299	A	19960816	ZA 1995-1299	19950216	<--
EP 745073	A1	19961204	EP 1995-910984	19950216	<--
EP 745073	B1	20000712			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
CN 1141038	A	19970122	CN 1995-191654	19950216	<--
BR 9506819	A	19970909	BR 1995-6819	19950216	<--
JP 09509174	T2	19970916	JP 1995-521868	19950216	<--
IL 112665	A1	19990509	IL 1995-112665	19950216	<--
IL 124139	A1	20000229	IL 1995-124139	19950216	<--
TW 384288	B	20000311	TW 1995-84101398	19950216	<--
AT 194608	E	20000715	AT 1995-910984	19950216	<--
ES 2149971	T3	20001116	ES 1995-910984	19950216	<--
HR 950070	B1	20010228	HR 1995-950070	19950216	<--
US 5633279	A	19970527	US 1995-483042	19950606	<--
FI 9603218	A	19961011	FI 1996-3218	19960816	<--

PRIORITY APPLN. INFO.:	US 1994-198749	A	19940218
	IL 1995-112665	A3	19950216
	WO 1995-US1787	W	19950216

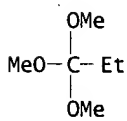
OTHER SOURCE(S): MARPAT 124:86709
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A pharmaceutical compn. comprising 5-substituted derivs. I of mycophenolic acid, where R1 = H, COR10, R10 = lower alkyl, aryl or NH-aryl; Z = CH2CH:CZ1CHZ2CZ3Z4COG, ZB, ZC, ZD, ZE, ZF, ZG, or ZH; Z1 = H, lower alkyl, halo, CF3; Z2 = H, OH, lower alkyl, lower alkoxy, aryl, or CH2Z13, Z13 = halo, CN, aryl, heteroaryl; Z3 = H, OH, lower alkyl, lower alkenyl, lower alkoxy, halo, Ph, P(O)(OMe)2, P(O)(OH)(OMe), NHZ11, SH, SOmZ12, Z11 = H, alkyl, acyl lower alkyl sulfonyl, Z12 = lower alkyl, m = 0-2; Z4 = H, OH, lower alkyl, halo, Ph, where Z4 is not OH or halo when Z3 = OH, halo, P(O)(OMe)2, P(O)(OH)(OMe), NHZ11, SZ12; Z3Z4 = cycloalkyl of 3-5 carbons; G = OH, lower alkoxy, lower thioalkyl, NG1G2, O(CH2)nNG1G2, O(CH2)nN:G3, n = 1-6, G1,G2 = H, lower alkyl, :G3 = lower alkylene of 4-6 carbons or of 3-5 carbons and one of O, S, NG4, G4 = H, lower alkyl; provided that when Z1 = Me, Z2, Z3 and Z4 are not all H and when R1, Z3, Z4 are all H and Z1 = Me, Z2 is not H or OH; for ZB, Z5 = H or lower alkyl; Z8 = H, lower alkyl or forms double bond with D2; D1D2 form a substituted or unsatd. or unsatd. carbocyclic or heterocyclic ring of 3-7 atoms; for ZC, Z8 = H or lower alkyl; for ZD, D3 = CH2 CH2CH2; for ZE, Z6 = H, lower alkyl, lower alkoxy, CO2H, NH2, N3, or halo; Z7 = H, lower alkyl, lower alkoxy, or halo; for ZH, D4 = (CH2)y, O, OCH2, y = 1-3. The disclosed hexenoic acid side-chain derivs. of mycophenolic acid are therapeutic agents advantageous in the treatment of disease states indicated for mycophenolic acid and/or mycophenolate mofetil, including immune, inflammatory, tumor, proliferative, viral or psoriatic disorders.

IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 5-substituted derivs. of mycophenolic acid as therapeutic agents for treatment of disease states)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



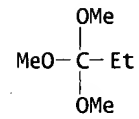
L30 ANSWER 15 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:982953 CAPLUS

DOCUMENT NUMBER: 124:117168
TITLE: Nonpeptide Angiotensin II Receptor Antagonists: Synthesis, Biological Activities, and Structure-Activity Relationships of Imidazole-5-carboxylic Acids Bearing Alkyl, Alkenyl, and Hydroxyalkyl Substituents at the 4-Position and Their Related Compounds
AUTHOR(S): Yanagisawa, Hiroaki; Amemiya, Yoshiya; Kanazaki, Takuro; Shimoji, Yasuo; Fujimoto, Koichi; Kitahara, Yoshiko; Sada, Toshio; Mizuno, Makoto; Ikeda, Masahiro; et al.
CORPORATE SOURCE: Research Institute, Sankyo Company Ltd., Tokyo, 140, Japan
SOURCE: Journal of Medicinal Chemistry (**1996**), 39(1), 323-38
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of imidazole-5-carboxylic acids bearing alkyl, alkenyl, and hydroxyalkyl substituents at the 4-position and their related compds. were prepd. and evaluated for their antagonistic activities to the angiotensin II (AII) receptor. Among them, the 4-(1-hydroxyalkyl)imidazole derivs. had strong binding affinity to the AII receptor and potently inhibited the AII-induced pressor response by i.v. administration. Various esters of these acids showed potent and long-lasting antagonistic activity by oral administration. The most promising compds. were (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl (CS-866) and (pivaloyloxy)methyl esters of 4-(1-hydroxy-1-methylethyl)-2-propyl-1-[(2'-1H-tetrazol-5-ylbiphenyl-4-yl)methyl]imidazole-5-carboxylic acid (I). A study involving stereochem. comparison of I with the acetylated C-terminal pentapeptide of AII was also undertaken.

IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, biol. activities, and structure-activity relationships of imidazole-5-carboxylic acids bearing alkyl, alkenyl, and hydroxyalkyl substituents at the 4-position and their related compds.)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 16 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:898965 CAPLUS
DOCUMENT NUMBER: 123:313962
TITLE: Method for producing imidazopyridine derivatives by cyclocondensation of 2,3-diaminopyridine with orthoesters
INVENTOR(S): Morisawa, Yoshitomi; Okazoe, Takashi; Yasuda, Arata
PATENT ASSIGNEE(S): Asahi Glass Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07138259	A2	19950530	JP 1993-187275	19930630 <--

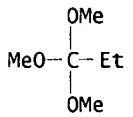
PRIORITY APPLN. INFO.: JP 1993-187275 19930630
OTHER SOURCE(S): CASREACT 123:313962; MARPAT 123:313962
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; X, Y = CH, N; R1, R2 = H, halo, lower (halo)alkyl or cycloalkyl, alkenyl, alkoxy, CmF2m+1, (CH2)nR5, (CH2)pCOR6; wherein m = 1-6; n = 1-4; p = 0-4; R5 = HO, alkoxy;R6 = H, HO, lower alkyl, alkoxy; R4 = monovalent arom. org. group bonded to CH2 through the C atom, e.g., Q - Q5; wherein R7, R8 = H, halo, lower alkyl, alkoxy, aralkyl, CkF2k+1; wherein k = 1-6; R9 = H, halo, HO, monovalent org. group], having angiotensin II-antagonizing and hypotensive activity and are useful as medicaments for diseases of the circulatory system such as hypertension (no data), are prepd. by cyclocondensation of 2,3-diaminopyridine (II; Z = H, lower alkyl, alkoxy, alkoxy-lower alkyl, aralkyl, acyl, alkoxycarbonyl, Bz; X, Y, R1, R2, R4 = same as above, in particular X = N, Y = CH, and Z = H) with R3CL1L2L3 (L1 - L3 = leaving group; or CL1L2 = CO or CS; R3 = same as above) in the presence of an acid catalyst such as HCl, H2SO4, HNO3, H3PO4, toluenesulfonic acid, or p-toluenesulfonic acid. This process smoothly gives I in good yields without undesired side effects. Thus, 0.42 g 2,3-diaminopyridine deriv. II (X = N, Y = CH, Z = H, R1 = 4-Me, R2 = 6-Me, R4 = Q6) (prepn. given) was dissolved in 1 mL DMF , followed by adding 3 mL tri-Me orthoformate and concd. 0.1 mL, and the resulting mixt. was stirred at room temp. for 18 h to give 0.30 g imidazol[4,5-b]pyridine deriv. (III; R4 = Q6).

IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of imidazopyridine derivs. by cyclocondensation of diaminopyridine with orthoesters as angiotensin II antagonists and antihypertensives)

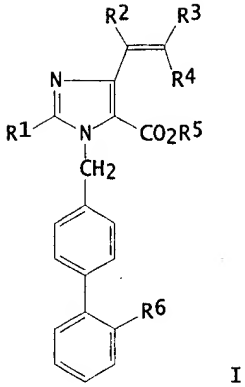
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 17 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:557640 CAPLUS
DOCUMENT NUMBER: 121:157640
TITLE: preparation of vinylimidazoles as antihypertensives
INVENTOR(S): Yanagisawa, Hiroaki; Amamya, Yosha; Kanezaki, Takuo; Shimoji, Yasuo; Koike, Hiroyuki; Sada, Toshio
PATENT ASSIGNEE(S): Sankyo Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 34 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06087833	A2	19940329	JP 1993-178652	19930720 <--

PRIORITY APPLN. INFO.: JP 1992-193762 19920721
OTHER SOURCE(S): MARPAT 121:157640
GI



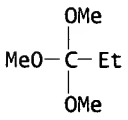
I

AB Title compds. I [R1 = C1-6 alkyl, C3-6 alkenyl, R7-X-A; R7 = C1-6 alkyl, C3-6 cycloalkyl; A = bond, C1-4 alkylene; X = O, S; R2, R3 = H, C1-6 alkyl, C3-6 cycloalkyl, C6-10 aryl, C7-13 aralkyl; R3R4 = C4-6 alkylene; R5 = H, protecting group; R6 = (protected) CO2H, tetrazol-5-yl] and their pharmaceutically acceptable salts, inhibitors of angiotensin II-induced hypertension, are prepd. E.g., a soln. of Et 4-isopropenyl-2-propylimidazole-5-carboxylate (prepn. given) and 4-[2-(trityltetrazol-5-yl)phenyl]benzyl bromide in DMF contg. KOCMe3 was stirred at room temp. for 1 h to give I [R1-R6 = Pr, Me, H, H, Et, tetrazol-5-yl], which was hydrolyzed to give the corresponding free acid, which had an ID50 of 0.012 i.v. for inhibiting angiotensin II-induced hypertension in rats.

IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepn. of antihypertensives)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 18 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:207924 CAPLUS

DOCUMENT NUMBER: 120:207924

TITLE: Angiotensin II receptor antagonists: imidazoles and pyrroles bearing hydroxymethyl and carboxy substituents

AUTHOR(S): Yanagisawa, Hiroaki; Amemiya, Yoshiya; Kanazaki, Takuro; Fujimoto, Koichi; Simoii, Yasuo; Fujimoto, Yoshiko; Sada, Toshio; Mizuno, Makoto; Koike, Hiroyuki

CORPORATE SOURCE: Res. Inst., Sankyo Co. Ltd., Tokyo, 140, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (**1994**), 4(1), 177-82
CODEN: BMCLE8; ISSN: 0960-894X

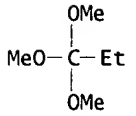
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Imidazoles and pyrroles bearing hydroxymethyl and carboxy groups were prepd., and their AII antagonistic activities were evaluated. The hydroxymethyl substituent at the 4 position and the carboxy substituent at the 5 position in the imidazole nucleus were favorable for the activity.

IT **24823-81-2**, Trimethyl orthopropionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diaminomaleonitrile)

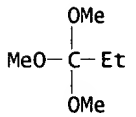
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 19 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:111521 CAPLUS
DOCUMENT NUMBER: 120:111521
TITLE: Hydrocarbon fuel composition
INVENTOR(S): Kanne, Diane D.
PATENT ASSIGNEE(S): Union Oil Co. of California, USA
SOURCE: U.S., 8 pp. Cont. of U.S. Ser. No. 671,570, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5268008	A	19931207	US 1990-611972	19901113 <--
PRIORITY APPLN. INFO.:			US 1982-453494	19821227
			US 1984-671570	19841115

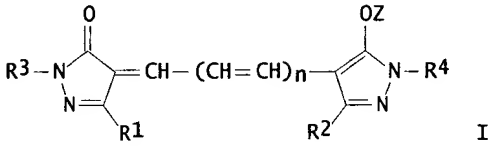
OTHER SOURCE(S): MARPAT 120:111521
AB Hydrocarbon fuels, esp. diesel fuel compns., contain orthoesters to reduce particulate emissions therefrom when combusted in an internal combustion engine.
IT **24823-81-2**, Trimethyl orthopropionate
RL: USES (Uses)
(diesel fuel additives, for control of particulate emissions)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 20 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:659420 CAPLUS
DOCUMENT NUMBER: 119:259420
TITLE: Microprecipitated methine oxonol filter dye dispersion for photographic material
INVENTOR(S): Texter, John
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

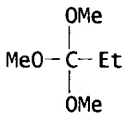
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 549486	A2	19930630	EP 1992-420455	19921211 <--
EP 549486	A3	19940420		

EP 549486 B1 19980715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
US 5274109 A 19931228 US 1991-812519 19911220 <--
JP 05265139 A2 19931015 JP 1992-338219 19921218 <--
US 5326687 A 19940705 US 1993-134342 19931008 <--
PRIORITY APPLN. INFO.: US 1991-812519 19911220
OTHER SOURCE(S): MARPAT 119:259420
GI



I

AB A Ag halide photog. material contains a micropptd. dispersion of a methine oxonol filter dye having the general formula I [R1-4 = (substituted) alkyl or aryl and .gtoreq.1 R1-4 contains CO2Z where Z+ is a statistical mixt. of H+ and M+ where M+ = an alkali metal or tetraalkylammonium cation such that Z+ = xH+ + (1-x)M+ where x = 0.33-0.95; n = 0, 1, or 2].
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepg. methine oxonol photog. filter dyes)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 21 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:512715 CAPLUS
DOCUMENT NUMBER: 117:112715
TITLE: Manufacture of unsaturated mono and dicarboxylic acid imides
INVENTOR(S): Yonemoto, Tatsuo; Saito, Eiichiro; Matsumura, Masahiro
PATENT ASSIGNEE(S): Matsushita Electric Works, Ltd., Japan
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

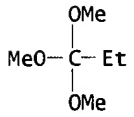
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5112989	A	19920512	US 1989-325807	19890320 <--
CA 1338809	A1	19961224	CA 1989-594134	19890317 <--

PRIORITY APPLN. INFO.: US 1989-325807 19890320
OTHER SOURCE(S): MARPAT 117:112715
AB The title compds. with purity >90%, useful in manuf. of addn.-type imide resins, are prepd. by esterification of unsatd. amic acids with ortho esters and imidation of the resulting amic acid ester. Thus, adding 4,4'-diaminodiphenylmethane-AcMe soln. in 1 h to maleic anhydride-AcMe soln., stirring the mixt. 2 h, adding water, filtering, water-washing, and drying gave a bisamic acid (I) with purity 98.5%. Heating a AcNMe2 contg. I and MeC(OMe)4 1 h at 80.degree., adding water, filtering, water-washing, and drying gave a bisamic acid ester (II) with purity 98%. Heating

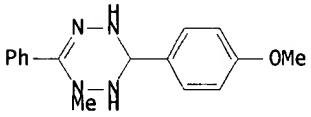
II-AcNMe2 soln. 2 h at 40.degree. and 10-3 mmHg, filtering, water-washing, and drying gave a bismaleimide with purity 97.5%.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of amic acids)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 22 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:151725 CAPLUS
DOCUMENT NUMBER: 116:151725
TITLE: Hydrazidines. V. Synthesis and reactions of aromatic and aliphatic hydrazidines and the N1-substituted derivatives
AUTHOR(S): Neunhoeffer, Hans; Karafiat, Ute; Koehler, Gernot; Sowa, Birgit
CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Germany
SOURCE: Liebigs Annalen der Chemie (**1992**), (2), 115-26
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 116:151725
GI

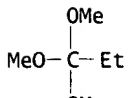


III

AB Arom. hydrazidines RC(:NNH2)NHNH2 (I, R = Ph, substituted Ph) were synthesized by reaction of arom. orthocarboxylates with tert-Bu carbazate and reaction of the protected hydrazidines with HCl/methanol or HBr/acetic acid. Aliph. N1-methylhydrazidines were prepd. by methylation of bis(tert-butyloxycarbonyl)hydrazidines and deprotection with HBr/acetic acid. Arom. N1-methylhydrazidines RC(:NNH2)NMeNH2 II (R = p-MeC6H4, p-ClC6H4, p-MeC6H4) were obtained by methylation of N1-methyl(thiohydrazides) followed by, reaction with tert-Bu carbazate and deprotection with HCl/methanol. Attempts to remove both protecting groups in N1-alkyl-N2,N4-bis(benzylidene)hydrazidines failed. Cyclocondensation reactions of I and II gave tetrazine and triazine derivs., e.g. III.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tert-butyl carbazate)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



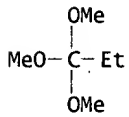
L30 ANSWER 23 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:187657 CAPLUS
DOCUMENT NUMBER: 114:187657
TITLE: Alkoxysilyl group-containing polymer coatings with good storage stability
INVENTOR(S): Kudo, Takezo; Aoki, Shoji
PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02284950	A2	19901122	JP 1989-108222	19890426 <--
JP 2875810	B2	19990331		

PRIORITY APPLN. INFO.: JP 1989-108222 19890426

AB The title compns. comprise 100 parts copolymers contg. unsatd. alkoxysilanes 0.5-50, comonomers 40-99.4%, and unsatd. carboxylic acids 0.1-10%; 0.5-30 parts orthopropionate and/or orthobutyrate esters, 5-50 parts C1-10 alkanols, and 0-500 parts pigments. Thus, a 50% soln. of polymer from Me methacrylate 400, Bu methacrylate 500, .gamma.-methacryloxypropyltrimethoxysilane 100, and maleic anhydride 5 parts contg. 2% EtC(OMe)3 (I) and 33 parts TiO2 had viscosity at 25.degree. 27 and 32 P after 0 and 1 mo, resp., at 50.degree.; vs. 27 and gelled, resp., without I.

IT **24823-81-2**, Trimethyl orthopropionate
RL: MOA (Modifier or additive use); USES (Uses)
(heat stabilizers, for acrylic polymer coating compns.)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 24 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:516595 CAPLUS
DOCUMENT NUMBER: 113:116595
TITLE: Alkoxysilyl-containing polymer compositions with improved storage stability
INVENTOR(S): Kudo, Takezo; Aoki, Shoji; Miyashita, Masahiko
PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 02058556	A2	19900227	JP 1988-13333	19880123 <--
JP 2631383	B2	19970716		

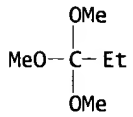
PRIORITY APPLN. INFO.: JP 1988-13333 19880123

AB The title compns. are composed of (A) 100 parts of copolymers comprising 0.5-50% alkoxysilyl-contg. vinyl monomers (I) and 50-99.5% other monomers copolymerizable with I, (B) 0.5-30 parts orthopropionate ester and/or ortholactate ester, and (C) 5-50 parts C1-10 alkyl alcs. Thus, Me methacrylate 400, Bu methacrylate 500, .gamma.-methacryloxypropyl trimethoxysilane 100, xylene 420, iso-PrOH 50, and Bz2O2 2 parts were heated at 90.degree. for 10 h to obtain a 50%-solids polymer soln., 100 parts of which was mixed with 5 parts tri-Me orthopropionate (II) and 500 ppm H2O. The mixt. showed viscosity (25.degree.) 1650 cP-s initially and 2360 cP-s after 1 mo in a sealed tube at 50.degree., vs. 2250 and gelled, resp., for a control compn. prepd. without II.

IT **24823-81-2**
RL: USES (Uses)
(alkoxysilyl-contg. polymer compns. contg., with good storage stability)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 25 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:490688 CAPLUS

DOCUMENT NUMBER: 113:90688

TITLE: Gas chromatographic assay for 3,9-diethylidene-2,4,8,10-tetraoxaspiro[5.5]undecane

AUTHOR(S): Pogany, Stefano A.; Deeken, Rodney A.; Zentner, Gaylen M.

CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., INTERx Res. Corp., Lawrence, KS, 66047, USA

SOURCE: Journal of Chromatography (**1990**), 508(1), 179-86
CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

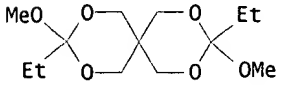
OTHER SOURCE(S): CASREACT 113:90688

AB A gas chromatog. method was developed, based on a ref. std. for anal. of the reactive diketene acetal 3,9-diethylidene-2,4,8,10-tetraoxaspiro[5.5]undecane (DETOSU). The method is based on the conversion of DETOSU to 3,9-diethyl-3,9-dimethoxy-2,4,8,10-tetraoxaspiro[5.5]undecane, a stable ortho ester. Cross-linked 100% Me silicone was used as the stationary phase. Six impurities were identified in the DETOSU by gas chromatog. and gas chromatog.-mass spectrometry.

IT **128672-11-7P**
RL: SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(prepn. and identification of, in diethylidenetetraoxaspiroundecane by gas chromatog.)

RN 128672-11-7 CAPLUS

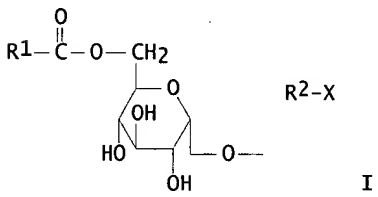
CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-diethyl-3,9-dimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 26 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:231899 CAPLUS
DOCUMENT NUMBER: 112:231899
TITLE: Preparation of oligoglucoside substrates for alpha-amylase determination
INVENTOR(S): Schmidt, Axel; Van der Eltz, Herbert; Rauscher, Elli
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H., Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

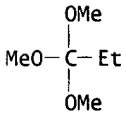
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 321871	A2	19890628	EP 1988-121068	19881216 <--
EP 321871	A3	19910612		
EP 321871	B1	19930707		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DE 3743908	A1	19890706	DE 1987-3743908	19871223 <--
AT 91284	E	19930715	AT 1988-121068	19881216 <--
ES 2058225	T3	19941101	ES 1988-121068	19881216 <--
ZA 8809431	A	19890927	ZA 1988-9431	19881219 <--
US 5068182	A	19911126	US 1988-288471	19881222 <--
AU 8827576	A1	19890629	AU 1988-27576	19881223 <--
AU 603941	B2	19901129		
JP 02138291	A2	19900528	JP 1988-323815	19881223 <--
JP 06055753	B4	19940727		

PRIORITY APPLN. INFO.: DE 1987-3743908 19871223
EP 1988-121068 19881216
OTHER SOURCE(S): MARPAT 112:231899
GI



I

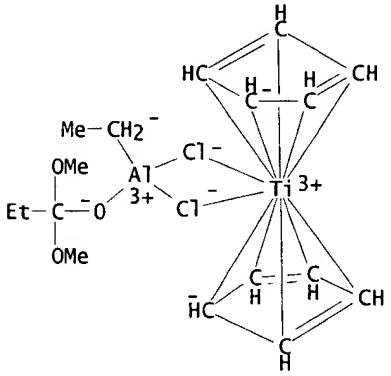
AB Oligoglucosides I [R1 = H, C1-4 alkyl, substituted C3-6 cycloalkyl, Ph, tetrahydropyranyl, (substituted) amino, etc.; R2 = oligoglucoside with 2-4 glucose units; X = H, chromogen] are prepd. as substrates for detn. of .alpha.-amylase activity. Thus, resorufin was refluxed with Ag2O in MeCN in the presence of a mol. sieve and absence of moisture, and acetobromo-.alpha.-D-maltopentaose was added to produce resorufinyl-.beta.-D-maltopentaose (II), which was esterified with an ortho ester to II isobutyrate. Incubation of this substrate with .alpha.- and .beta.-glucosidases and human serum contg. .alpha.-amylase produced a marked increase in absorbance at 578 nm.
IT **24823-81-2**
RL: BIOL (Biological study)
(in substrate prepn. for amylase detn.)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 27 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:39095 CAPLUS
DOCUMENT NUMBER: 110:39095
TITLE: EPR spectra of products of the reaction of di-.eta.5-cyclopentadienyl(diethylalanedi-.mu.-chloro)titanium(III) with C1 compounds
AUTHOR(S): Tyrlik, S. K.; Korda, A.; Poppe, L.; Rockenbauer, A.; Gyoer, M.
CORPORATE SOURCE: Inst. Org. Chem., Pol. Acad. Sci., Warsaw, 00-961, Pol.
SOURCE: Journal of Organometallic Chemistry (1987), 336(3), 343-8
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:39095

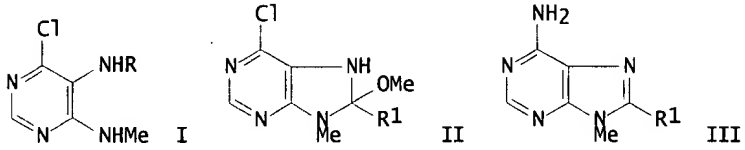
AB The outcome of the reaction of di-.eta.5-cyclopentadienyl(diethylalanedi-.mu.-chloro)titanium(III) (I) with MeOH depends strongly on the molar ratio: with I/MeOH < 0.75 the methanol cleaves the Al-Et bond; with higher ratios solvated Cp2TiCl (Cp = cyclopentadienyl) is formed. The compds. HCHO, CO2, HCONH2, HCO2Me and (MeO)2CO react with I at the Al-Et bond to give new paramagnetic dimers independent of the molar ratio. The chlorinated species CHnCl4-n (n = 0-2) either oxidized titanium(III) to titanium(IV) or give unidentified paramagnetic species.

IT **118229-11-1P**
RL: PRP (Properties); PREP (Preparation)
(formation and ESR spectra of)
RN 118229-11-1 CAPLUS
CN Titanium, di-.mu.-chlorobis(.eta.5-2,4-cyclopentadien-1-yl)[(1,1-dimethoxy-1-propanolato)ethylaluminum]- (9CI) (CA INDEX NAME)



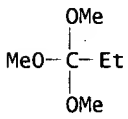
L30 ANSWER 28 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:7922 CAPLUS
DOCUMENT NUMBER: 110:7922
TITLE: Synthesis of 8-alkyl derivatives of 9-methyladenine
AUTHOR(S): Draminski, Marcin; Frass, Elzbieta
CORPORATE SOURCE: Inst. Basic Sci., Mil. Sch. Med., Lodz, 90647, Pol.
SOURCE: Polish Journal of Chemistry (1987), 61(7-12), 901-6

CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:7922
GI



I II III

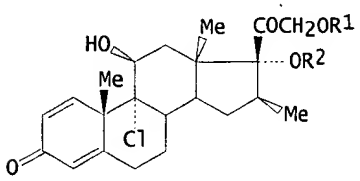
AB Reaction of the aminopyrimidine I (R = H) with R1C(OMe)3 (R1 = Me, Et, Pr, Bu) gave the dihydropurines II which on ammonolysis gave the methyladenines III. Treatment of I (R = H) with (R1CO)2O gave I (R = R1CO) which on ammonolysis also gave III.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminochloropyrimidine)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 29 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1988:132168 CAPLUS
DOCUMENT NUMBER: 108:132168
TITLE: Process for the preparation of 9.alpha.-chloro-11.beta.-hydroxy-16.beta.-methyl-1,4-pregnadiene-3,20-dione 17-propionate 21-(2-hydroxybenzoate), useful as an antiinflammatory agent
INVENTOR(S): Gonzalez Bosch, Jose Maria; Gris Seoane, Pedro J.
PATENT ASSIGNEE(S): Laboratorios Menarini S. A., Spain
SOURCE: Span., 13 pp.
CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 538692	A1	19870416	ES 1984-538692	19841217 <--

PRIORITY APPLN. INFO.: ES 1984-538692 19841217
GI



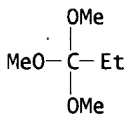
I

AB The antiinflammatory (no data) title steroid (I; R1 = COC6H4OH-2, R2 = COEt) (II) is prepd. from I (R1 = R2 = H) (III) via I (R1 = H, R2 = COEt) (IV). A soln. of EtC(OMe)3 in dioxane was added to a mixt. of III and pyridinium tosylate catalyst in C6H6/dioxane at <40.degree.. The mixt. was refluxed for 18-20 h and partially evapd. in vacuo, and the residue was hydrolyzed with 0.1M acetate buffer (4 h reflux). Evapn., pptn. in ice water, and crystn. from 4:1 MeOH/Me2CO gave IV. Subsequent conversion of IV to II by treatment with 2-AcOC6H4COCl and selective acid hydrolysis is not exemplified.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with trihydroxypregnadienedione deriv.)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 30 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1988:132167 CAPLUS

DOCUMENT NUMBER: 108:132167

TITLE: Process for preparing 17-esters of 9.alpha.-chloro-11.beta.,17.alpha.,21-trihydroxy-16.beta.-methyl-1,4-pregnadiene-3,20-dione, useful as antiinflammatory agents or their intermediates

INVENTOR(S): Gonzalez Bosch, Jose Maria; Gris Seoane, Pedro J.

PATENT ASSIGNEE(S): Laboratorios Menarini S. A., Spain

SOURCE: Span., 9 pp.
CODEN: SPXXAD

DOCUMENT TYPE: Patent

LANGUAGE: Spanish

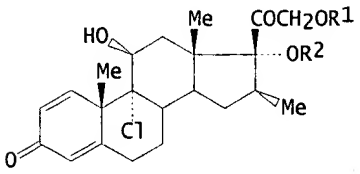
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 550677	A1	19870301	ES 1986-550677	19860103 <--

PRIORITY APPLN. INFO.: ES 1986-550677 19860103

GI

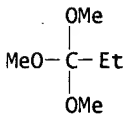


I

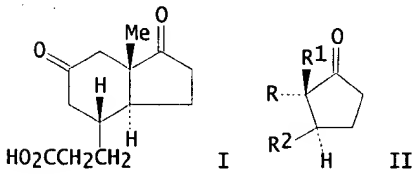
AB The antiinflammatory title ester I (R1 = COC6H4OH-2, R2 = COEt) (II) is prepd. from I (R1 = R2 = H) (III) in 3 steps. Treatment of III with EtC(OMe)3 and pyridinium tosylate catalyst, followed by hydrolytic workup, gives I (R1 = H, R2 = COEt; IV) (no example). A soln. of 2-AcOC6H4COCl in dioxane was added to a soln. of IV in pyridine/dioxane, and the mixt. was stirred 8-10 h at 10-15.degree. and pptd. in ice water to give I (R1 = COC6H4OAc-2, R2 = COEt) (V). Selective hydrolysis of 0.1 mol V in THF by dropwise addn. of 1M NaOH in MeOH (0.08 mol total) at <25.degree. gave II.

IT **24823-81-2**

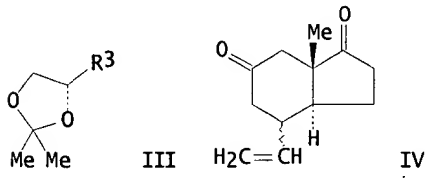
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with trihydroxypregnadienedione deriv.)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 31 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1987:515270 CAPLUS
DOCUMENT NUMBER: 107:115270
TITLE: Enantioselective synthesis of trans-octahydro-1,6-dioxoinden-4-ylpropionic acid from (R)-2,3-O-isopropylideneglyceraldehyde by tandem orthoester Claisen rearrangement
AUTHOR(S): Suzuki, Toshio; Sato, Etsuko; Unno, Katsuo; Kametani, Tetsuji
CORPORATE SOURCE: Dep. Pharm., Akita Univ. Hosp., Akita, 010, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1986**), (12), 2263-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:115270
GI



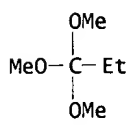
I II



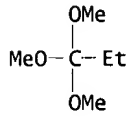
III IV

AB The title compd. I was prepd. via the methylcyclopentanone II (R = Me, R1 = H, R2 = HOCH2CH:CH), which was constructed by consecutive ortho ester Claisen rearrangements of isopropylidenedioxypentenol III [R3 = CH(OH)CH:CH2] and (6S,4E)-Me3CSiMe2OCH2CH(OH)CH:CHCH2CH2CO2Me derived from III (R3 = CHO). Methylvinylhexahydroindenediones IV, possessing trans ring fusion, were prepd. by Dieckman condensation of II (R = MeO2CCH2, R1 = Me, R2 = MeO2CCH2CHCH:CH2) which were prepd. by the regio- and stereoselective alkylation of II (R = Me, R1 = H, R2 = HOCH2CH:CH) and then ortho ester Claisen rearrangement of II (R = MeO2CCH2, R1 = Me, R2 = HOCH2CH:CH).
IT **24823-81-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and Claisen rearrangement of, with Me (dimethylbutylsilyloxy)hydroxyheptenoate)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)

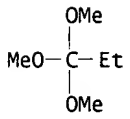


L30 ANSWER 32 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:496815 CAPLUS
DOCUMENT NUMBER: 105:96815
TITLE: Stereoselective acid-catalyzed Claisen rearrangements
AUTHOR(S): Daub, G. William; Shanklin, Paula L.; Tata, Claudia
CORPORATE SOURCE: Dep. Chem., Harvey Mudd Coll., Claremont, CA, 91711, USA
SOURCE: Journal of Organic Chemistry (1986), 51(17), 3402-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:96815
AB An alkyl substituent in the 2-position of an (E)-trisubstituted allylic alc. confers significant diastereoselectivity on acid-catalyzed Claisen rearrangement of the system. Syn/anti ratios of 5:1 are obsd. for both ortho ester and ketal Claisen rearrangement, which had previously shown very little diastereoselectivity. The selectivity is ascribed to the presence of a 1-3 diaxial-like interaction in the transition state leading to the anti isomer, an interaction absent in that leading to the syn isomer.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with allylic alcs., diastereoselectivity in)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 33 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:50503 CAPLUS
DOCUMENT NUMBER: 104:50503
TITLE: Thermochemical studies of carbonyl compounds. 3. Enthalpies of hydrolysis of ortho esters
AUTHOR(S): Wiberg, Kenneth B.; Martin, Eric J.; Squires, Robert R.
CORPORATE SOURCE: Dep. Chem., Yale Univ., New Haven, CT, 06511, USA
SOURCE: Journal of Organic Chemistry (1985), 50(24), 4717-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The hydrolysis enthalpies (.DELTA.Hr) of ortho esters are detd. in aq. dioxane. The largest effect on .DELTA.Hr was found with .alpha.-branching, in contrast to the previously reported hydrolysis of ketals which gave the larger effect with .beta.-branching. Possible

reasons for this difference in behavior are discussed.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, heat of)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 34 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1985:405917 CAPLUS
DOCUMENT NUMBER: 103:5917
TITLE: Facile synthesis of alkoxyalkyl cyclopentadienes
AUTHOR(S): Sternbach, Daniel D.; Hobbs, Sheila H.
CORPORATE SOURCE: Dep. Chem., Duke Univ., Durham, NC, 27706, USA
SOURCE: Synthetic Communications (**1984**), 14(14), 1305-12
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:5917
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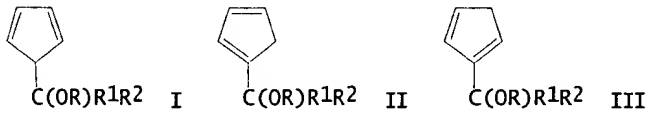
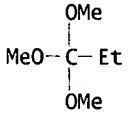
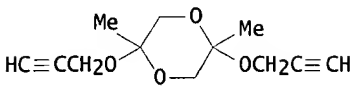


AB Mixts. of alkylated cyclopentadienes I, II, and III (R = Me, Et; R1 = OMe, OEt, alkyl, alkenyl; R2 = H, alkyl) were prepd. from 5-(trimethylsilyl)cyclopentadiene (IV), R1C(OR)2R2, and CF3SO3SiMe3. IV was treated with HC(OMe)3 and CF3SO3SiMe3 at room temp. to give I (R = Me, R1 = OMe, R2 = H), II (R = Me, R1 = OMe, R2 = H) (major product), and III (R = Me, R1 = OMe, R2 = H).
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted condensation of, with (trimethylsilyl)cyclopentadiene, catalysts for)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



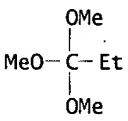
L30 ANSWER 35 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1984:510836 CAPLUS
DOCUMENT NUMBER: 101:110836
TITLE: Catalytic conversion of propargyl alcohol and its derivatives
AUTHOR(S): Matnishyan, A. A.; Grigoryan, S. G.; Panosyan, G. A.; Arutyunyan, A. V.; Davtyan, M. M.; Mardoyan, M. K.;

Nikogosov, V. N.
CORPORATE SOURCE: VNII "IREA", Yerevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1984), 37(4), 233-7
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

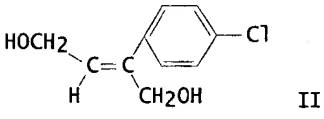


II

AB Treating abs. HC.tplbond.CCH2OH (I) with HgO 4 h at 40.degree. yields 29.5% Hg(C.tplbond.CCH2OH)2. A mixt. of I and HgO-BF3.OEt2 kept 5 h at 22.degree. gave 57% II. Similarly obtained was 43% MeOCH2C(OMe)2Me from MeOCH2C.tplbond.CH. A mechanism for cyclodimerization is discussed.
IT **24823-81-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from Me propargyl ether)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



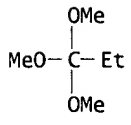
L30 ANSWER 36 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1984:454636 CAPLUS
DOCUMENT NUMBER: 101:54636
TITLE: A new synthesis of trans-2-substituted-2-butene-1,4-diols from 2-butyne-1,4-diol via nucleophilic addition of Grignard reagents
AUTHOR(S): Ishino, Yoshio; Wakamoto, Kohji; Hirashima, Tsuneaki
CORPORATE SOURCE: Osaka Munic. Tech. Res. Inst., Osaka, 536, Japan
SOURCE: Chemistry Letters (1984), (5), 765-8
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:54636
GI



II

AB trans-2-Substituted-2-butene-1,4-diols were readily obtained by reactions of 2-butyne-1,4-diol (I) with Grignard reagents in good yields. E.g., treating I with 4-ClC6H4MgBr gave 85% butenediol II.
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Grignard reagent and butynediol)

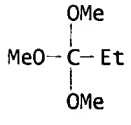
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 37 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1983:559035 CAPLUS
DOCUMENT NUMBER: 99:159035
TITLE: Catalysts for olefin polymerization
INVENTOR(S): Martin, Joel L.
PATENT ASSIGNEE(S): Phillips Petroleum Co. , USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

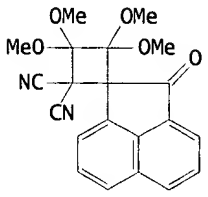
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4400303	A	19830823	US 1981-241975	19810309 <--
US 4442277	A	19840410	US 1982-421222	19820922 <--

PRIORITY APPLN. INFO.: US 1981-241975 19810309
AB Ethylene polymers are prepd. in the presence of catalysts prepg. by pretreating solid particles of Mg dihalides by copulverizing in the presence of acetals, ketals, or orthoesters, and reacting the pretreated particles with a Ti halide. Thus, 15 g MgCl2 was ballmilled 16 h with 2.68 g CH(OEt)3 [122-51-0], and 2.00 g of the product was treated with 3.45 g TiCl4 in 5 mL hexane at 23.degree. for 1 h to give a catalyst. A reactor contg. 0.0240 g above catalyst, 1.2 L isobutane, and 3 mmols AlEt3 [97-93-8] was heated to 80.degree., pressurized with ethylene to 0.69 MPa, and pressurized with ethylene to maintain pressure at 2.1 MPa to give 1217 g polyethylene [9002-88-4] (catalyst productivity 50.7 kg polymer/g catalyst).
IT **24823-81-2**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polymn. of ethylene)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)

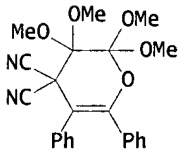


L30 ANSWER 38 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1983:422264 CAPLUS
DOCUMENT NUMBER: 99:22264
TITLE: Chemistry of ketene acetals. VI. The influence of the dicyanoethene moiety on the reactivity and selectivity of .beta.,.beta.-dicyano-.alpha.,.beta.-unsaturated ketones in cycloadditions with ketene acetals
AUTHOR(S): Bakker, C. G.; Ooms, P. H. M.; Scheeren, J. W.; Nivard, R. J. F.
CORPORATE SOURCE: Dep. Org. Chem., Catholic Univ., Nijmegen, 6525 ED,

Neth.
SOURCE: Recueil: Journal of the Royal Netherlands Chemical Society (1983), 102(3), 130-5
CODEN: RJRSDK; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



III

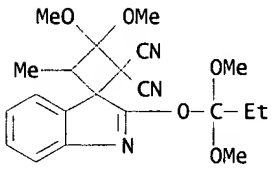


IV

AB The (2 + 2) vs. (4 + 2) cycloaddns. of ketene acetals R1R2C:C(OMe)2 (I; R1 = R2 = OMe; R1 = H, R2 = Me) with .beta.,.beta.-dicyano-.alpha.,.beta.-unsatd. ketones R3COR3C:C(CN)2 (II; R3 = R4 = Ph; R3R4 = o-COC6H4, o-C6h4C6H4-o 1,8-naphthylenediyl, o-C6H4NH) were investigated. Cyclobutanes, e.g. III, were only obtained at room temp. in the cycloaddn. of II (R3 = R4 = Ph) with I (R1 = R2 = OMe) and II (R3R4 = 1,8-naphthylenediyl) with I (R1 = R2 = MeO; R1 = H, R2 = Me). In the latter case, an oxetane was obtained when ZnCl2 was used as a catalyst. The thermodynamically more stable (4 + 2) cycloadducts, e.g. IV, were obtained at higher temps., except from II (R3R4 = o-C6H4NH) in which the carbonyl group is part of an amide function. A high regiospecificity was found in these cycloaddns. The influence of the dicyanoethene moiety on the cycloaddns. is discussed and compared to analogous cycloaddns. of I with .alpha.,.beta.-unsatd. ketones and .alpha.-diketones.

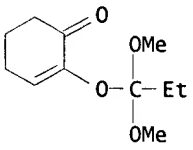
IT **86143-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 86143-70-6 CAPLUS
CN Spiro[cyclobutane-1,3'-[3H]indole]-2,2-dicarbonitrile, 2'-(1,1-dimethoxypropoxy)-3,3-dimethoxy-4-methyl- (9CI) (CA INDEX NAME)

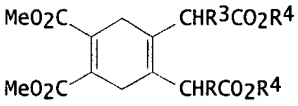


L30 ANSWER 39 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1983:159962 CAPLUS
DOCUMENT NUMBER: 98:159962
TITLE: Chemistry of ketene acetals V. Catalyzed and noncatalyzed [2 + 2]- and [4 + 2]-cycloadditions between 1,2-diketones and ketene acetals
AUTHOR(S): Bakker, C. G.; Scheeren, J. W.; Nivard, R. J. F.
CORPORATE SOURCE: Dep. Org. Chem., Catholic Univ. Nijmegen, Nijmegen, 6525 ED, Neth.
SOURCE: Recueil: Journal of the Royal Netherlands Chemical Society (1983), 102(2), 96-102
CODEN: RJRSDK; ISSN: 0165-0513
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:159962
AB Generally, 1,1-dimethoxypropene (I) yields only [2 + 2]-cycloadducts, viz. oxetanes and bisoxetanes, in reactions with 1,2-diketones; [4 + 2]-cycloaddn. products, viz. dihydrodioxins, are not formed because of their thermodn. instability. In similar reactions of tetramethoxyethene (II), dihydrodioxins, however, are obtained, when the [4 + 2]-cycloaddn. is accompanied by an increase in the stabilization energy of the diketone moiety. The difference between I and II can be ascribed to the low .pi.-bond energy of II.
IT **85291-27-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 85291-27-6 CAPLUS
CN 2-Cyclohexen-1-one, 2-(1,1-dimethoxypropoxy)- (9CI) (CA INDEX NAME)

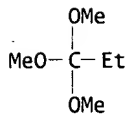


L30 ANSWER 40 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1982:615493 CAPLUS
DOCUMENT NUMBER: 97:215493
TITLE: A new synthesis of 3,4-bis[methylene]-hexanedioic esters from 2-butynediol via Claisen orthoester rearrangement
AUTHOR(S): Ishino, Yoshio; Nishiguchi, Ikuzo; Kim, Michiaki; Hirashima, Tsuneaki
CORPORATE SOURCE: Osaka Munic. Tech. Res. Inst., Osaka, 530, Japan
SOURCE: Synthesis (**1982**), (9), 740-2
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:215493
GI



II

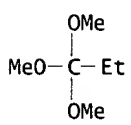
AB The reaction of HOCH2C.tplbond.CCH2OH (I) with RCHR1C(OR2)3 (R = H, Me, Et, Cl, CH2CN, Ph, p-tolyl, 4-ClC6H4, p-anisyl; R1 = H, Me; R2 = Et, Me) gave R2O2CCRR1C(:CH2)C(:CH2)CRR1CO2R2. A mixt. of I, MeC(OEt)3, and EtCO2H was heated at 110.degree. to give EtO2CCH2C(:CH2)C(:CH2)CH2CO2Et. The Diels-Alder reaction of MeO2CC.tplbond.CCO2Me with 3,4-dimethyleneadipate esters gave cyclohexadienes II (R3 = H, Ph; R4 = Et, Me).
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sym. butynediol)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 41 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1982:35909 CAPLUS
DOCUMENT NUMBER: 96:35909
TITLE: Polymerization of .alpha.-olefins
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc. , Japan
SOURCE: Belg., 16 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 888581	A1	19810817	BE 1981-204617	19810427 <--
JP 57031906	A2	19820220	JP 1980-107120	19800806 <--
JP 63038365	B4	19880729		

PRIORITY APPLN. INFO.: JP 1980-107120 19800806
AB Catalysts for the stereospecific polymn. of olefins are prepd. by grinding Mg halides with (cyclo)aliph. orthoesters (ratio 1:0.01-0.15) and treating the products with Ti halides. Thus, MgCl2 and MeC(OEt)3 (mol ratio 1:0.052) are ball-milled for 40 h, and 10 g this product and 50 mL TiCl4 are stirred 2 h at 80.degree., decanted, and washed to give a solid contg. 1.71% active Ti. Stirring 100 mg this solid and AlEt3 0.20, Et2AlCl 0.18, and Me p-toluate 0.12 mL in 1 L heptane with 0.1 kg/cm2 H and 5 kg/cm2 C3H6 at 70.degree. for 2 h gives 253 g polypropylene [9003-07-0] (2614 g/g active Ti catalyst) with boiling heptane-sol. content 5.5%, bulk d. 0.34, and limiting viscosity index (Tetralin, 135.degree.) 1.52, and 8.4 g heptane-sol. polymer.
IT **24823-81-2D**, reaction products with magnesium chloride and titanium tetrachloride
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for stereospecific polymn. of olefins)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)

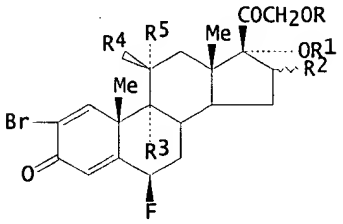


L30 ANSWER 42 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:569600 CAPLUS
DOCUMENT NUMBER: 95:169600
TITLE: 2-Bromo-6 -fluoro-3-keto-.DELTA.1,4-pregnanes
INVENTOR(S): Palladino, Gaetano
PATENT ASSIGNEE(S): Italy
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3041774	A1	19810521	DE 1980-3041774	19801105 <--
JP 55154998	A2	19801202	JP 1979-61382	19790518 <--
FR 2469418	A1	19810522	FR 1980-23601	19801105 <--
FR 2469418	B1	19830708		
BE 886045	A1	19810302	BE 1980-202711	19801106 <--
CH 645390	A	19840928	CH 1980-8257	19801106 <--
NL 8006114	A	19810601	NL 1980-6114	19801107 <--
GB 2065660	A	19810701	GB 1980-35829	19801107 <--

PRIORITY APPLN. INFO.:
IT 1979-27098 19791107
GB 1974-10443 19740308
GB 1977-43231 19740308
DE 1980-3041774 19801105

GI



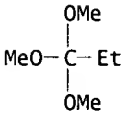
I

AB Title steroids I (R = H, acyl; R1 = H, C2-8 acyl; R2 = H, HO, Me; R3 = F, Cl; R4 = HO, Cl, R5 = H; R4R5 = O) were prepd. Thus, bromination of 15 g 6.beta.,9.alpha.-fluoroprednisolone 17,21-diacetate in peroxide free dioxene by Br gave 14.3 g I (R = R1 = Ac, R2 = R5 = H, R3 = F, R4 = OH).

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of bromodifluoropregnadienetrioldione)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



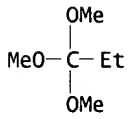
L30 ANSWER 43 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:514842 CAPLUS
DOCUMENT NUMBER: 95:114842
TITLE: .beta.,.beta.-Diacyl enamines and enols. Part 6. Efficient synthesis of aminoalkylidene derivatives of five-membered ring active methylene compounds
AUTHOR(S): Wolfbeis, Otto S.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria
SOURCE: Monatshefte fuer Chemie (**1981**), 112(3), 369-83
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Tri-Me orthoacetate, -propionate, or -benzoate, in contrast to orthoformate, do not undergo a 3 component condensation with anilines and cyclic 6-membered active methylene compds. to the corresponding N-substituted aminomethylene derivs.; they do react, however, with 5-membered ring compds. The reaction proceeds smoothly with primary aliph. or arom. amines, whereas secondary amines give no or only low

yields. In comparison to other synthetic routes to .beta.,.beta.-diacyl enamines the condensation described has the following advantages: (a) the products thus obtained have previously often required a 2-step procedure, (b) the only reaction product besides the aminoalkylidene deriv. is an alc., (c) the usually mild conditions allow the prepn. of compds. so far not available by employing more drastic alternative methods.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with amines and 5-membered ring active methylene compds.)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 44 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:586559 CAPLUS
DOCUMENT NUMBER: 93:186559
TITLE: Pesticidally active salts and compositions containing them
INVENTOR(S): Baillie, Alister Cameron; Wright, Brian John; Wright, Kenneth
PATENT ASSIGNEE(S): Fisons Ltd., UK
SOURCE: Eur. Pat. Appl., 73 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

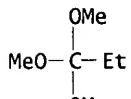
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 9348	A2	19800402	EP 1979-301805	19790903 <--
EP 9348	A3	19801001		
EP 9348	B1	19830720		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4339443	A	19820713	US 1979-70440	19790828 <--
AT 4158	E	19830815	AT 1979-301805	19790903 <--
BR 7905980	A	19800527	BR 1979-5980	19790919 <--
JP 55045685	A2	19800331	JP 1979-120942	19790921 <--
CA 1140566	A1	19830201	CA 1979-336145	19790921 <--

PRIORITY APPLN. INFO.: GB 1978-37723 19780922
GB 1978-45140 19781118
EP 1979-301805 19790903

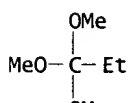
AB Approx. 50 title compds. such as RCOP(X)R1R2 (R = H, alkyl, alkenyl, alkynyl, aryl; R1 = R, RO; R2 = OR3, NR3R4, R3 = 1 equiv. of an agriculturally acceptable cation such as Na or Li, R3, R4 = H, alkyl; X = O, S) were prepd. E.g., 0.066 mol AcP(O)(OMe)2 and 0.1 mol NaI gave 9.5 g AcP(O)(OMe)(ONa). Also prepd. were Me(CH2)4(EtCO)P(O)ONa, HOCH2(PrCO)P(O)OLi, and Na methyl(2-methyl-1,3-thiazolidin-2-yl)phosphinate (I). At 1.4 kg/ha, I showed 100% post emergent herbicidal activity against Barnyard grass and Crabgrass after 21 days.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with Me phosphonous dichloride)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 45 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:549192 CAPLUS
DOCUMENT NUMBER: 93:149192
TITLE: Effect of the acyl substituent on the equilibrium constant for hydration of esters
AUTHOR(S): Guthrie, J. Peter; Cullimore, Patricia A.
CORPORATE SOURCE: Dep. Chem., Univ. West. Ontario, London, ON, N6A 5B7, Can.
SOURCE: Canadian Journal of Chemistry (1980), 58(13), 1281-94
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Heats of hydrolysis were measured for the tri-Me orthoesters of isobutyric, propionic, benzoic, methoxyacetic, chloroacetic, and cyanoacetic acids by using aq. acid with an org. cosolvent where necessary, and of the corresponding esters in alk. soln. Solubilities or free energies of transfer from gas to aq. soln. were measured, permitting calcn. of the free energies of formation of the aq. orthoesters, and calcn. of the free energies of formation of the covalent hydrates of the esters, and the free energy changes for hydration of these esters. By using estd. pKa values equil. consts. were calcd. for the addn. of hydroxide to the esters. The data are in good agreement with the appropriate Marcus equation relating rate and equil. consts. with a value for b of 8.99 .+-. 0.17. This line was used to est. the equil const. for addn. of hydroxide, and thence of water, to some addnl. esters where only the rate const. was available. Rate consts. for hydrolysis of Me esters in aq. soln. at 25.degree. were calcd. from literature data, correcting for the effect of other conditions as necessary. From the equil. consts. for addn. of water, rate consts. were estd. for uncatalyzed hydrolysis; for the cases where this rate const. was measured, the agreement was satisfactory. For acid catalyzed hydrolysis the data permit a test of the 2 alternative mechanisms considered previously, namely specific acid catalysis and general acid catalysis with hydronium ion acting as a general acid. For esters the mechanism is clearly specific acid catalysis, but for aldehydes and ketones it appears very likely that the mechanism is general acid catalysis.
IT **24823-81-2**
RL: PRP (Properties)
(hydrolysis and hydration of, mechanism and thermodn. of)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 46 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:76142 CAPLUS
DOCUMENT NUMBER: 92:76142
TITLE: cis-2-Benzoyl-3-hydroxy-2-alkenonitriles as antiinflammatory agents
INVENTOR(S): Hanifin, John W., Jr.; Ridge, David N.

PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 4173650	A	19791106	US 1978-957595	19781103	<--
ZA 7904124	A	19800827	ZA 1979-4124	19790808	<--
WO 8000964	A1	19800515	WO 1979-US610	19790815	<--
W: JP					
JP 55500866	T2	19801030	JP 1979-501792	19790815	<--
EP 11910	A2	19800611	EP 1979-301687	19790817	<--
EP 16277	A1	19801001			
EP 16277	B1	19811202			
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE					
CA 1130298	A1	19820824	CA 1979-334092	19790820	<--
AU 7952452	A1	19800508	AU 1979-52452	19791102	<--
AU 532753	B2	19831013			
EP 35284	A3	19811007	EP 1981-102641	19810408	<--
EP 35284	A2	19810909			
EP 35284	B1	19830713			
R: BE, CH, DE, FR, GB, IT, NL, SE					

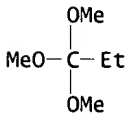
PRIORITY APPLN. INFO.:

US 1978-957595	19781103
US 1978-968899	19781213
US 1979-34315	19790430
WO 1979-US610	19790815
EP 1979-301687	19790817

AB cis-MOCR:C(CN)COR1 (M = H or pharmaceutically acceptable cation, e.g., Tl; R = C1-4 alkyl; R1 = Ph, optionally substituted by halo, CF3, CCl3, or C1-4 alkyl or alkoxy), having antiinflammatory activity which made them useful for treating arthritis, were prepd. Thus, condensation of 4-FC6H4COCH2CN with MeC(OMe)2NMe2:C(CN)COC6H4F-4, which, at 25 mg/kg, gave 65% inhibition of swelling in adjuvant-induced arthritis in rats.

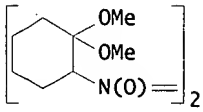
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (fluorobenzoyl)acetonitrile)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)

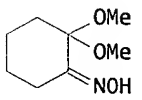


L30 ANSWER 47 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1979:86809 CAPLUS
DOCUMENT NUMBER: 90:86809
TITLE: Nitrosation in organic chemistry. General synthesis of .alpha.-nitroso ketone acetal dimers and .alpha.-oximino ketone acetals and mechanism of their fragmentation reactions
AUTHOR(S): Klein, Karl P.; Demmin, Timothy R.; Oxenrider, Bryce C.; Rogic, Milorad M.; Tetenbaum, Marvin T.
CORPORATE SOURCE: Corp. Res. Cent., Allied Chem. Corp., Morristown, NJ, USA
SOURCE: Journal of Organic Chemistry (1979), 44(2), 275-85
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal

LANGUAGE: English
GI



I

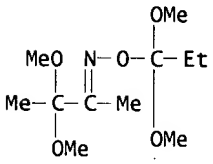


II

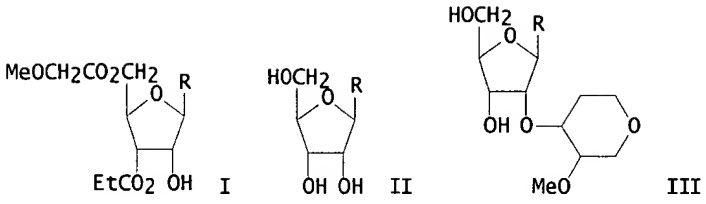
AB Treating 1-methoxycyclohexene with MeONO in SO2 soln. contg. H2SO4, BF3-Et2O or other acid catalyst, or more effectively, in excess MeONO as solvent, gave the dimer I in essentially quant. yield. Other cyclic and open chain enol ethers were similarly converted into .alpha.-nitroso ketone acetal dimers, which on heating gave the corresponding .alpha.-oximino ketone acetals, e.g., II. The oximino ketone acetals react with ortho esters to give adducts, which in the presence of an acid catalyst provide a carbonium ion that undergoes rapid fragmentation. E.g., II was converted into NC(CH2)4CO2Me (III) by treatment with HC(OMe)2 and then MeSO3H in CCl4. I underwent fragmentation to III more readily than did II, which suggests that the previously discussed nitrosolysis reaction involves fragmentation of the .alpha.-nitroso ketone acetal monomer and not .alpha.-oximino ketone acetal.

IT **68226-31-3**
RL: PROC (Process)
(fragmentation of)

RN 68226-31-3 CAPLUS
CN 2-Butanone, 3,3-dimethoxy-, O-(1,1-dimethoxypropyl)oxime (9CI) (CA INDEX NAME)



L30 ANSWER 48 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:7266 CAPLUS
DOCUMENT NUMBER: 88:7266
TITLE: General method for the synthesis of 3',5'-diesters and 2'-acetals of the four common nucleosides
AUTHOR(S): Van Boom, J. H.; Burgers, P. M. J.; Haasnoot, C. A. G.; Reese, C. B.
CORPORATE SOURCE: Gorlaeus Lab., Univ. Leiden, Leiden, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1977), 96(4), 91-5
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

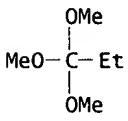


AB A procedure for the prepn. of 5'-O-(methoxyacetyl)-3'-O-propionylribonucleosides I (R = uracil-1-yl, 4-N-p-anisoylcytosin-1-yl, 6-N-p-anisoyladenin-9-yl, 2-N-benzoylguanin-9-yl) from the ribonucleosides II was developed. The usefulness of I as starting products for the synthesis of cryst. 2'-O-(methoxytetrahydropyranyl)-ribonucleosides III, which are key intermediates in the synthesis of oligoribonucleotides, was demonstrated.

IT **24823-81-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with nucleosides)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 49 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:502308 CAPLUS

DOCUMENT NUMBER: 87:102308

TITLE: Hydroxy-2-alkoxy-1,3-benzodioxoles

INVENTOR(S): Eicken, Karl; Huber, Rolf

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

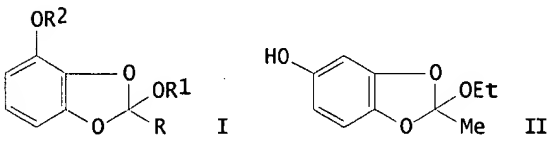
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2550965	A1	19770526	DE 1975-2550965	19751113 <--

PRIORITY APPLN. INFO.: DE 1975-2550965 19751113

GI



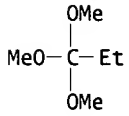
AB Benzodioxoles I (R = Me, Et, R1 = Me, R2 = H; R = CH2Cl, R1 = Et, R2 = H) were prepd. by condensing pyrogallol with RC(OR1)3. II was similarly

prepd. Reaction of I (R = CH2Cl, R1 = Et, R2 = H; R = Et, R1 = Me, R2 = H) with MeNCO gave I (R2 = CONHMe) which at 0.05 mg gave 80-100% mortality among Blatta orientalis.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with pyrogallol)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 50 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:171388 CAPLUS

DOCUMENT NUMBER: 86:171388

TITLE: Organic electrosyntheses. IX. Condensation of 2-aminophenylhydrazine with ortho esters

AUTHOR(S): Falsig, Mogens; Iversen, Palle E.

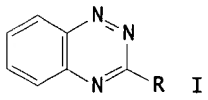
CORPORATE SOURCE: Dep. Org. Chem., Univ. Aarhus, Aarhus, Den.

SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1977), B31(1), 15-20
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

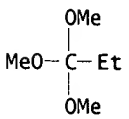


AB 2-H2NC6H4NHNH2 was prepd. in high yield by large-scale cathodic redn. of benzotriazole in acidic medium. 3-Substituted benzo-1,2,4-triazines I (R = H, Me, Et, Ph) were prepd. by condensation of 2-H2NC6H4NHNH2 with ortho esters. The optimum conditions for this reaction were found from kinetic measurements and variation of the reaction parameters, detg. the product concn. by means of cathodic DC-polarography.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aminophenylhydrazine, benzotriazine deriv. from, kinetics for)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 51 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1975:531336 CAPLUS

DOCUMENT NUMBER: 83:131336

TITLE: N1-(Alkoxyalkylidene)-3,5-dinitrosulfanilamides

PATENT ASSIGNEE(S): Lilly, Eli, and Co., USA
SOURCE: Austrian, 11 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

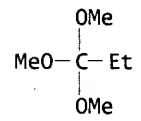
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 315147	B	19740510	AT 1972-3308	19720414 <--

PRIORITY APPLN. INFO.: AT 1972-3308 19720414

AB 4,3,5-(Pr2N)(O2N)2C6H2SO2N:C(OR)R1 (I; R = Me, Et, Pr, Bu, H2C:CHCH2, etc.; R1 = H, Me, Et, Ph) were prepd. by the reaction of 4,3,5-(Pr2N)(O2N)2C6H2SO2NH2(II) with an ortho ester. Thus, II was heated with MeC(OEt)3 to give I (R = Et, R1 = Me). I were useful as herbicides and were tested on various plants.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dinitrodipropylsulfanilamide)

RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 52 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:443544 CAPLUS
DOCUMENT NUMBER: 83:43544
TITLE: Farnesylacetic acid esters and 2-substituted derivatives for pharmaceuticals
INVENTOR(S): Fujita, Yoshiji; Omura, Yoshiaki; Nishida, Takashi; Itoi, Kazuo
PATENT ASSIGNEE(S): Kuraray Co., Ltd.
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

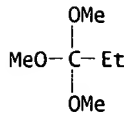
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2431811	A1	19750130	DE 1974-2431811	19740702 <--
DE 2431811	C2	19821028		
JP 50029518	A2	19750325	JP 1973-79448	19730713 <--
JP 56023415	B4	19810530		
GB 1451173	A	19760929	GB 1974-28178	19740625 <--
CH 592601	A	19771031	CH 1974-9659	19740712 <--
FR 2241530	A1	19750321	FR 1974-24522	19740715 <--

PRIORITY APPLN. INFO.: JP 1973-79448 19730713

AB Reaction of nerolidol with the appropriate trialkyl orthoacetate in the presence of a catalytic amt. of aliph. carboxylic acid (e.g., isobutyric, butyric, oxalic acid) at .apprx.125-45.degree. for 8-48 hr gave 87.2-94.2% (Z,Z)-Me2C:CH(CH2CH2CMe:CH)2CH2CHRCO2R1 (R = H, R1 = Me, Et, Pr, Bu, cyclohexyl; R = R1 = Me; R = Et, Ph, cyclohexyl, R1 = Et).

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nerolidol)

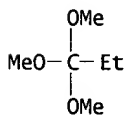
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 53 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:86565 CAPLUS
DOCUMENT NUMBER: 82:86565
TITLE: Acyl derivatives of proscillaridin A
INVENTOR(S): Loesel, Walter; Merz, Herbert
PATENT ASSIGNEE(S): Boehringer, C. H., Sohn
SOURCE: Ger. Offen., 16 pp. Division of Ger. Offen. 2,063,406 (CA 77: 165040r).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2065628	A1	19741205	DE 1970-2065628	19701223 <--
DE 2065628	C3	19791206		
DE 2065628	B2	19790419		

PRIORITY APPLN. INFO.: DE 1970-2065628 19701223
GI For diagram(s), see printed CA Issue.
AB Treatment of proscillaridin A (I) with orthoesters gave 14 II [R1 = Pr2CO, PhCO, EtCO, Cl(CH2)3CO, cyclopropyl-, cyclopentyl-, cyclohexyl-, and cyclooctylcarbonyl-, R2 = H], which reacted with acid chlorides to give the 4'-acyl deriv. or with MeI to give the 4'-O-alkyl deriv. Thus, I reacted with EtC(OMe)3 in THF contg. p-MeC6H4SO3H to give II (R1 = Et2CO, R2 = H), which reacted with EtCOCl in pyridine to give II (R1 = R2 = Et2CO) or with MeI to give II (R1 = Et2CO, R2 = Me). II have a pos. inotropic effect and are useful in treating heart insufficiency (no data).
IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with proscillaridin A)
RN 24823-81-2 CAPLUS
CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 54 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1973:432186 CAPLUS
DOCUMENT NUMBER: 79:32186
TITLE: Antiinflammatory 6.alpha.,9.alpha.-difluoro-21-deoxyprednisolone esters
INVENTOR(S): Gardi, Rinaldo; Vitali, Romano; Falconi, Giovanni
PATENT ASSIGNEE(S): Warner-Lambert Co.
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
DE 2256129	A1	19730524	DE 1972-2256129	19721116	<--
DE 2256129	B2	19800717			
DE 2256129	C3	19811105			
US 3763196	A	19731002	US 1972-306636	19721114	<--
CA 976155	A1	19751014	CA 1972-156365	19721114	<--
GB 1395775	A	19750529	GB 1972-52687	19721115	<--
SE 385122	B	19760608	SE 1972-14849	19721115	<--
NL 7215563	A	19730522	NL 1972-15563	19721117	<--
NL 165470	B	19801117			
NL 165470	C	19810415			
FR 2160659	A1	19730629	FR 1972-41036	19721117	<--
DK 127781	B	19740107	DK 1972-5742	19721117	<--
CH 579102	A	19760831	CH 1972-16798	19721117	<--
JP 48061466	A2	19730828	JP 1972-116128	19721118	<--
JP 51025024	B4	19760728			
AU 7249715	A1	19740606	AU 1972-49715	19721206	<--

PRIORITY APPLN. INFO.: IT 1971-31368 19711119

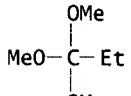
GI For diagram(s), see printed CA Issue.

AB The title compds. [I, R = Ph (II), Et, or Pr] were prepd. and used as local inflammation inhibitors. Thus, 5 g 6.alpha.,9-difluoroprednisolone and PhC(OMe)3 were refluxed in dioxane and C6H6 in the presence of pyridine for 1 hr with removal of the solvent to give 5.5 g 6.alpha.,9-difluoro-11.beta.-hydroxy-17,21-(.alpha.-methoxybenzylidenedioxy)pregna-1,4-diene-3,20-dione (III). III (2 g) was refluxed in MeOH in the presence of aq. AcONa at pH 3.9 for 2 hr to give 1.45 g IV (R = Ph). IV (R = Ph) (10 g) was treated with p-MeC6H4SO3H in pyridine and CH2Cl2 overnight at 0-5.degree. to give 13 g V (R = Ph), which was refluxed successively with NaI in Me2CO for 24 hr and with AcOH for 1 hr to give 8.5 g II.

IT **24823-81-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 6.alpha.,9-difluoroprednisolone-17-propionate)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 55 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1964:52297 CAPLUS

DOCUMENT NUMBER: 60:52297

ORIGINAL REFERENCE NO.: 60:9140e-f

TITLE: Orthopropionic acid trialkyl esters

AUTHOR(S): Zaretskii, V. I.

SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) **(1964)**, 37(1), 218-20
CODEN: ZPKHAB; ISSN: 0044-4618

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

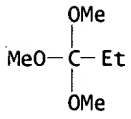
AB cf. U.S.S.R. 105,467, CA 52, 1207a. Orthocarboxylic acid trialkyl esters were prepd. under conditions suitable for production. A mixt. of 0.8 mole propionitrile, 0.8 mole abs. alc., and 200 cc. dry CHCl3 was satd. with dry HCl to a content of 7.5-8% (phenolphthalein) and kept 3 days at .ltoreq.0.degree.. Abs. alc. (100 g.) was added to the mixt. at -5.degree., excess HCl detd. (bromphenol blue), the mixt. neutralized with EtONa soln. (7% Na, n g. alc.) portionwise (Congo), 84 - n g. abs. alc. added, the mixt. stirred 9 hrs. at 39-42.degree., cooled to 0.degree., filtered, the ppt. washed with abs. alc., the filtrate washed with 10%

Na2CO3, and the org. layer dried (K2CO3), filtered, and distd. to give 38-49% EtC(OEt)3. The following esters were prepd. similarly: EtC(OMe)3, EtC(OPr)3 (b5.5-6 79-80.5.degree., b2 54-5.degree., n20D 1.4145, d20 0.8689), and EtC(OBu)3 (b1.5 93.5-6.5.degree., 103.5.degree., n20D 1.4230, d20 0.8713) in 55-60, 34, and 39% yield, resp. The starting compds. must not contain >0.1% H2O.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester
(prepn. of)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 56 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1954:33747 CAPLUS

DOCUMENT NUMBER: 48:33747

ORIGINAL REFERENCE NO.: 48:6051g-i

TITLE: Acetylene solution

INVENTOR(S): Walker, Harry M.

PATENT ASSIGNEE(S): Monsanto Chemical Co.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

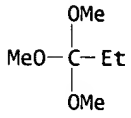
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2666742		19540119	US	<--

AB Trimethyl esters of ortho aliphatic acids having the formula R-C.tplbond. (OMe)3, where R represents H or an alkyl radical contg. 1-3 C atoms, were found to be excellent solvents for C2H2 (I). High Bunsen coeffs. (the vol. of gas measured at 0.degree. and 1 atm. and dissolved at the temp. of the expt. in 1 vol. of solvent at a gas partial pressure of 1 atm.) for I in solvents indicate their excellent solvent action for I. The Bunsen coeff. detd. for trimethyl orthoformate is 15.12 and for trimethyl orthoacetate is 13.78. Trimethyl orthopropionate and trimethyl orthobutyrate are also suitable solvents. These solvents can be used in the extn. of I from dil. solns. of I, for storing I under elevated pressures, and in mixts. with other solvents for I.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester
(as solvent for C2H2)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 57 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1954:7013 CAPLUS

DOCUMENT NUMBER: 48:7013

ORIGINAL REFERENCE NO.: 48:1259b-i,1260a-c

TITLE: Ketene acetals. XXVII. The bromination of various ketene acetals

AUTHOR(S): McElvain, S. M.; Davie, Wm. R.

CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of the American Chemical Society (1952), 74, 1816-21
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

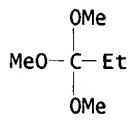
AB Monosubstituted ketene acetals, RCH:C(OR')2 [R = Me, R' = Et (I)] [R = Ph, R' = Me (II)] [R = CN, R' = Me (III)], when added to a soln. of Br in CCl4 at 0-5.degree. yield the corresponding bromo esters, RCHBrCO2R', (IV), (V), and (VI), and R'Br. A reverse order of mixing causes I and II to follow the reaction 2RCH:C(OR')2 + Br2 .fwdarw. R'Br + RCHBrC(OR')2CHRCO2R' (VII) and (VIII). VII and VIII are readily converted by pyrolysis to the tetronic acid enol ethers (IX) and (X). Under certain conditions, bromination of II yields di-Me .alpha.,.alpha.'-diphenylsuccinate (XI); possible reactions to account for XI are discussed. III follows a different bromination course to yield CNCBr:C(OMe)2 (XII). Me2C:C(OMe)2 (XIII), which yields only Me .alpha.-bromoisobutyrate regardless of the method of bromination, is converted in part to Me2CBrC(OMe)3 (XIV) when brominated in the presence of an orthoester. A mechanism for the reaction is shown. Bromination of CH2:C(OEt)2 (XV) is complicated by the ease of polymerization of XV; the only pure products that could be isolated were CH2BrCO2Et (XVI) and CHBr2CO2Et (XVII). PrCOCHMeCO2Et (7.25 g.) in Et2O at 0.degree. treated with 7.5 g. Br [Conrad and Schmidt, Ber. 29, 1043(1896)] yielded 8.8 g. Et .alpha.-methyl-.alpha.-bromo-.beta.-oxovalerate (XVIII), b0.2 58-62.degree., n25D 1.4550. XVIII (7 g.) refluxed 2 hrs. in 10% HBr, the soln. neutralized with NaHCO3, extd. with CHCl3, the aq. phase acidified and extd. with Et2O yielded 3 g. 3,5-dimethyltetronic acid (XIX), m. 123-4.degree.; phenylhydrazone, m. 188-91.degree.. 3,5-Diphenyltetronic acid (XX), m. 203-6.degree.. XX (3 g.) in 100 cc. dioxane treated with excess CH2N2 in Et2O, the mixt. let stand 30 min. at 5.degree., aerated, 10 cc. water, 10 cc. EtOH and a small amt. of NaHCO3 added to the residue, and the EtOH evapd., the aq. mixt. estd. with Et2O yielded a product (XXI), m. 117-18.degree., and XI, m. 84-6.degree.. Acid or basic hydrolysis of XXI yielded XX; XXI is 2-methoxy-3,5-diphenyl-4-oxo-4,5-dihydrofuran. For the bromoesters prepd., the compd., % yield, b.p./mm., and n25D are: IV, 86, 46-7.degree./9, 1.4430; V, 90, 133-7.degree./14, 1.5502; VI, 92, 88-93.degree./9, 1.4712; Me2CBrCO2Me (XXIIA), 92, 41-5.degree./11, 1.4480; XVI, 34, 45-50.degree./9, 1.4492. I (39 g.) at 0.degree. treated during 8 hrs. with 27 g. Br in 100 cc. CCl4 yielded 26 g. EtBr, 11.2 g. IV, and 36 g. VII, b0.2 86-90.degree., n25D 1.4538. VII (4 g.) heated 5 min. at 200.degree. yielded 1.8 g. IX, b15 147-50.degree., n25D 1.4720, d25 1.074. IX (4.5 g.) heated with 20 cc. 10% HBr yielded 2.3 g. XIX. XIX (4 g.) and 5 g. H2C(COEt)2 held 30 min. at 80.degree. and distd. yielded 3 g. VII, b25 155-7.degree., n25D 1.4740. Br absorption by II depended on the temp. and the rate of addn. of Br. II (74 g.) and 55.5 g. Br yielded 68.5 g. II and a residue which on distn. at 160-70.degree. and 0.05-0.1 mm. gave 4.3 g. XI, m. 165-70.degree.. XI on sapon. yielded the acid, m. 179-80.degree., solidified, and m. 226-8.degree.. At 185-90.degree. the product was XX Me ester, m. 85-6.degree.. The residue yielded an inert solid, m. 300-5.degree. (decompn.). PhBrCHCO2Me (33 g.) and 23 g. II heated 1 hr. at 150.degree. yielded 31 g. of a mixt. of meso- and dl- XI, m. 173-203.degree.. VIII (14 g.), 30 cc. EtOH, 30 cc. water, and 10 g. KOH refluxed 1 hr., the EtOH distd., and the residue acidified with 20 cc. HCl yielded XX, m. 203-6.degree.. III (43.2 g.) in 50 cc. CHCl3 at -10 to -20.degree. treated with 50 cc. of 61 g. Br made up to 100 cc. with CHCl3, the temp. let rise to 0.degree. 12 cc. of the soln. added, and the solvent removed in vacuo yielded NCCH2CO2Me, n25D 1.4170; Br(NC)CHCO2Me, n25D 1.4712; and 41% XII. XII (15 g.), 5 cc. water, 20 cc. dioxane, and 1 cc. AcOH let stand overnight at room temp. yielded 11.5 g. VI, b9 89-91.degree., n25D 1.4718. XII (15.5 g.) in 10 cc. CHCl3 with 12.9 g. Br in 15 cc. CHCl3 yielded 17.8 g. Me dibromocyanoacetate, b0.5 58-62.degree., n25D 1.5037. XIII in CCl4 treated with Br in CCl4 at 0.degree. yielded 89% XXIIA. XIII (24 g.) and EtC(OMe)3 at 0.degree. treated with 33 g. Br made up to 50 cc. with CHCl3 during 1 hr. yielded 12.5 g. EtC(OMe)3, 16.1 g. XXIIA, and 24.2 g. XIV, b18 77-9.degree., n25D 1.4510, m. about 25.degree.; the distillate yielded 7 g. EtCO2Me. XIII

(8.4 g.) and 8.4 g. Me2CHC(OMe)3 in 10 cc. CHCl3 at 0-5.degree. treated with 11.6 g. Br made up to 25 cc. in CHCl3 yielded 1.6 g. Me2CHC(OMe)3; 2.4 g. XXIIA, and 9.9 g. of a mixt. of XXIIA and XIV. XIV (5.4 g.) in 10 cc. 10% HBr let stand 1 hr. at room temp. yielded 3.6 g. XXIIA, b8 34-8.degree.. XV (15 g.) in 10 cc. CHCl3 at -78.degree. under N treated with 3 drops of 30% Br in CHCl3 and the mixt. heated 1 hr. at 150.degree. and 8 mm. yielded 4.5 g. polymer. XV (50 g.) in 10 cc. CCl4 at 50-60.degree. treated with 55 g. Br and the product distd. yielded (a) 20 g. BrCH2CO2Et, b9 43-7.degree., n25D 1.4493; (b) 3 g., b9 52-69.degree., n25D 1.4681; (c) 9.9 g., Br2CHCO2Et, b9 69-72.degree., n25D 1.4910; (d) 2.6 g., b9 79-108.degree., n25D 1.4800; (e) 3.2 g., b9 108-15.degree., n25D 1.4640; (f) 4 g., b0.3 74-8.degree., n25D 1.4635; (g) 1.2 g., b0.4 83-8.degree., n25D 1.4740; (h) 5.4 g., b0.4 91-100.degree., n25D 1.4965. The mixt. of products contained about 11 g. EtOAc. II (20.5 g.) treated with O (temp. held below 60.degree.) yielded 4.5 g. OC(OMe)2, m. -1.degree., n25D 1.3761; 5.1 g. BzH, b10 53.degree., n25D 1.5212; 4.9 g. of a mixt. of BzOMe and PhCH2CO2Me, b0.4 up to 90.degree.; and 7 g. XI; 1.5 g. tar remained.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester (prepn. of)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 58 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1951:13691 CAPLUS

DOCUMENT NUMBER: 45:13691

ORIGINAL REFERENCE NO.: 45:2400b-f

TITLE: Ketene acetals. XXI. The dealcoholation of orthoesters. Dimethylketene dimethylacetal

AUTHOR(S): McElvain, S. M.; Venerable, James T.

CORPORATE SOURCE: Univ. of Wisconsin, Madison

SOURCE: Journal of the American Chemical Society (1950), 72, 1661-9
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

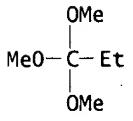
AB cf. C.A. 43, 3356f. Details are given of the prepn. of PhCH2C(OMe)3 (I), b0.5 72-6.degree., n25D 1.4948, 46%; the crude I (contg. 19% PhCH2CO2Me) (57 g.) was heated 5 hrs. with 5 g. NaH in 15 ml. petr. ether and distd. to give pure I. iso-PrCN (138 g.) in 90 ml. anhyd. MeOH and 750 ml. ether, treated with 78 g. dry HCl, gives 99% Me isobutyrimidate-HCl, which yields 43% Me orthoisobutyrate (II), b. 135-6.degree., d254 0.9253, n25D 1.4003, camphorlike odor. PhCCl3 and MeONa in MeOH, allowed to stand overnight and refluxed 4 hrs., give 86% Me orthobenzoate, b26 114-15.degree., d254 1.0637, n25D 1.4858. EtNa (4.8 g. Na) in 25 ml. petr. ether and 40 g. Et2Hg, treated (15 min.) with 15 g. I in petr. ether, give 10.6 g. of a mixt. contg. 74% PhCH:C(OMe)2 (III) and 26% I; 52% C2H6 is evolved. II and the other aliphatic orthoesters yielded no ketene acetal with EtNa. I does not react with Ph3CNa (74% recovery); C10H7Na reacts readily and exothermically but the C10H8 could not be sepd. from the other reaction products. PhCH2CH:CHNa, BuLi, iso-PrMgBr, and tert-BuMgBr with I give varying yields of III. 2,4,6-Me3C6H2MgBr (IV) and I give III (contg. crude 52% III, 8.8% PhCH2CO2Na), and 86% C6H3Me3. IV and EtC(OMe) give 54% MeCH:C(OMe)2 (V). II and IV, heated after removal of the ether, give 15.6% dimethylketene di-Me acetal (VI), b. 103-5.degree., n25D 1.4046; II in MeOH, refluxed 1 hr. with a little concd. HCl, gives unchanged II and iso-PrCO2Me. II does not react with BuLi. I and (MeO)3Al, heated about 20 min. at 210.degree., give 92% III and MeOH. I and Al2O3, heated at

175-210.degree., give 31% III, 54% PhCH2CO2Me, MeOH, and ether. II, passed over (MeO)3Al at 290-300.degree., gives only 8.6% VI. EtC(OMe)3 and (MeO)3Al at 240-50.degree. give 15% V and 54% unchanged ester.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester
(prepn. of)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L30 ANSWER 59 OF 59 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1936:15256 CAPLUS

DOCUMENT NUMBER: 30:15256

ORIGINAL REFERENCE NO.: 30:2005f-i,2006b-i,2007a-d

TITLE: Cyanine dye series. II. Carbocyanines with substituents in the three-carbon chain

AUTHOR(S): Brooker, L. G. S.; White, Frank L.

SOURCE: Journal of the American Chemical Society (1935), 57, 2480-8
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

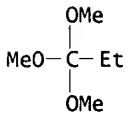
AB cf. C. A. 29, 2954.5. Ortho esters of higher aliphatic, of substituted aliphatic and of aromatic acids can be employed for the prepn. of thiacarbocyanines. These esters were prepd. by the action of an alc. upon an imino ester-HCl, prepd. in turn from a nitrile. Me orthopropionate (I), b. 126-8.degree. (69% yield in 6 days); Me orthobutyrate (II), b. 145-7.degree., 13%, 28 days; Me orthovalerate (III), b. 167-70.degree., 12%, 28 days; Me orthocaproate (IV), b. 187-90.degree., 40%, 5 days; Me orthoisocaproate (V), b. 178-81.degree., 9%, 35 days; Et orthophenoxyacetate (VI), b1.5 99-100.degree., 30%, 28 days; Et orthobenzoate (VII), b. 239.5-40.5.degree., 20%, 43 days. The intermediate imino ester-HCl salts were unstable, decompg. with evolution of gas and were converted directly into the ortho esters. 1-Methylbenzothiazole propiodide (VIII), m. 173-5.degree., 82% on heating 72 hrs. under reflux; butiodide (IX), m. 186-7.degree., 63% after 72 hrs.; alliodide (X), m. 192-3.degree., 88% after 20 hrs.; metho-p-toluenesulfonate (XI), m. 183.5-4.5.degree., 90% after 3 hrs. at 100.degree.; 1-methyl-.alpha.-naphthothiazole metho-p-toluenesulfonate (XII), m. 232-3.degree., 88% after 48 hrs. at 105-10.degree.; 2-methyl-.beta.-naphthothiazole metho-p-toluenesulfonate (XIII), m. 189-90.degree., 940% on heating 3 hrs. at 140.degree. and 3 days at 100.degree.. The quaternary salts were condensed with the ortho esters in boiling anhyd. C5H5N, the period of heating varying from 10 to 90 min. The yields are of the purified dye; all melt with decompn. Thiacarbocyanine iodides. 2,2'-diallyl, from X and HC(OEt)3 (XIV), bright, bronze needles, m. 264-6.degree., 77%; 2,2'-di-Pr, from VIII and XIV, prisms reflecting green and purple, m. 296-7.degree., 87%; 2,2'-di-Bu, from IX and XIV, dark purplish felt, m. 275-7.degree., 77%; 2,2'-diallyl-8-methyl, dark crystals with purplish reflex, m. 267-8.degree., 64% from X and MeC(OEt)3 (XV); 8-methyl-2,2'-dipropyl, purplish bronze, m. 295-6.degree., 64% from VIII and XV; 2,2'-dibutyl-8-methyl, dark crystals, reflecting blue and purple, m. 236-7.degree., 64% from IX and XV; 8-ethyl-2,2'-dimethyl, green reflex, m. 286-7.degree., 56% from 1-methylbenzothiazole-MeI (XVI) and EtC(OEt)3 (XVII); 2,2',8-tri-Et, double blue and green reflex, m. 236-7.degree., 41% from 1-methylbenzothiazole-EtI (XVIII) and XVII; 2,2'-diallyl-8-ethyl, green, m. 214-16.degree., 30% from X and XVII; 8-ethyl-2,2'-dipropyl, green, m. 248-50.degree., 28% from VIII and XVII; 2,2'-dibutyl-8-ethyl, dark prisms, reflecting purple and brilliant bronze, m. 241-3.degree., 28%

from IX and XVII; 2,2'-dimethyl-8-propyl, purple, m. 268-9.degree., 50% from XI and II; 2,2'-diethyl-8-propyl, greenish bronze, m. 246-8.degree., 55% from 1-methylbenzothiazole etho-p-toluenesulfonate (XIX) and II; 8-butyl-2,2'-dimethyl, purple with blue reflex, m. 168-9.degree., 42% from XI and III; 8-butyl-2,2'-diethyl, pale bronze, m. 233-4.degree., 58% from XIX and III; 8-amyl-2,2'-dimethyl, brown needles with very brilliant blue reflex, m. 217-19.degree., 55% from XI and IV; 8-amyl-2,2'-dimethyl, greenish bronze, m. 237-8.degree., 53% from XIX and IV; 8-isoamyl-2,2'-dimethyl, purplish brown with green reflex, m. 241-2.degree., 47% from XI and V; 8-isoamyl-2,2'-diethyl, double blue and green reflex, m. 219-20.degree., 51% from XIX and V; 8-benzyl-2,2'-dimethyl, reddish brown, m. 288-9.degree., 15% from XI and PhCH2C(OEt)3 (XX); 8-benzyl-2,2'-diethyl, emerald-green, m. 242-3.degree., 11% from XIX and XX; 2,2'-diallyl-8-benzyl, greenish blue, m. 225-7.degree., 33% from X and XX; 2,2'-dimethyl-8-PhOCH2, purplish brown, m. 255-7.degree., 48% from XI and VI; 2,2'-dimethyl-8-PhOCH2, reddish copper, m. 202-4.degree., 39% from XIX and VI; 2,2'-diallyl-8-PhOCH2, green, m. 211-13.degree., 41% from XI and VII; 2,2'-dimethyl-8-phenyl, bronze, m. 275-7.degree., 56% from XI and VII; 2,2'-diethyl -8- phenyl, greenish bronze, m. 300-1.degree., 56% from XIX and VII. 5,6,5',6'-Dibenzothiacarbocyanine bromides. 2,2'-di-Me , dark purplish felted mat, m. 285.degree., 83% from XII and XIV; 2,2'-di-Et, dark green, m. 280.degree., 68% from 1-methyl-.alpha.-naphthothiazole etho-p-toluenesulfonate (XXI) and XIV; 2,2',8-tri-Me, emerald-green, m. 278-81.degree., 42% from XII and XV; 2,2'-diethyl-8-methyl, greenish bronze, m. 261.degree., 43% from XXI and XV; 8-ethyl-2,2'-dimethyl, purple with blue reflex, m. 299.degree., 54% from XII and I; 2,2',8-tri-Et, greenish bronze, m. 296.degree., 37% from XXI and I; 2,2'-dimethyl-8-phenyl, dull purple, m. 308-10.degree., 37% from XII and VII; 2,2'-diethyl-8-phenyl, dull purple, m. 296.degree., 38% from XXI and VII. 3,4,3',4'-Dibenzothiacarbocyanine bromides. 2,2'-di-Me, greenish bronze, m. 237.degree., 73% from XIII and XIV; 2,2',8-tri-Me, lustrous green, m. 240-1.degree., 19% from XIII and XV; 8-ethyl-2,2'-dimethyl, green, m. 230.degree., 24% from XIII and XVII; 2,2',8-tri-Et, greenish bronze reflex, m. 247.degree., 29% from 2-methyl-.beta.-naphthothiazole etho-p-toluenesulfonate (XXII) and XVII; 2,2'-dimethyl-8-phenyl, greenish brown, m. 242-4.degree., 3% from XIII and VII; 2,2'-diethyl-8-phenyl, green, m. 252.degree., 4.5% from XXII and VII. Selenacarbocyanine iodides. 2,2',8-tri-Me, bluish purple, m. 290-1.degree. 36% from 1-methylbenzoselenazole metho-p-toluenesulfonate (XXIII) and XV; 8-ethyl-2,2'-dimethyl, green, m. 271-2.degree., 32% from XXIII and XVII; 2,2',8-tri-Et, double blue and brassy-green reflex, m. 146-8.degree. 16% from 1-methylbenzoselenazole etho-p-toluenesulfonate (XXIV) and XVII; 2,2'-dimethyl-8-phenyl, greenish bronze, m. 271-2.degree., 18% from XXIII and XIII; 2,2'-diethyl-8-phenyl, metallic greenish prisms, m. 280-1.degree., 13% from XXIV and VII. Oxacarbocyanine iodide. 2,2',8-tri-Me, garnet-red, m. 290-2.degree., 6% from 1-methylbenzoxazole metho-p-toluenesulfonate (XXV) and XV; 8-ethyl-2,2'-dimethyl, orange-red, m. 280-2.degree., 11% from XXV and XVII; 2,2',8-tri-Et, orange-red, m. 269-70.degree., 8% from 1-methylbenzoxazole ethiodide and XVII. Substitution of H in the mol. of a thiacarbocyanine dye derived from 1-methylbenzothiazole by an 8-Me group causes the absorption max. in MeOH to shift about 150 A. toward the blue but replacement of 8-Me by 8-Et shifts the max. about 50 A. back toward the red. Replacement of 8-Et by higher aliphatic groupings up to Am and iso-Am causes no further shift. Replacement of H by 8-benzyl causes a shift (75 A.) toward the blue but replacement by 8-Ph causes a slight shift (25 A.) toward the red. Somewhat similar relationships to those summarized above can be traced in the 3,4,3',4' and 5,6,5',6'-dibenzothiacarbocyanine series and in the selenacarbocyanines. The oxacarbocyanines are exceptional.

IT **24823-81-2**, Orthopropionic acid, trimethyl ester
(prepn. of)

RN 24823-81-2 CAPLUS

CN Propane, 1,1,1-trimethoxy- (9CI) (CA INDEX NAME)



L14 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2002 ACS
AN 1999:518292 CAPLUS
DN 131:161634
TI PEG-poly(**ortho ester**), PEG-poly(**ortho ester**)-PEG, and poly(**ortho ester**)-PEG-poly(**ortho ester**) block copolymers
IN Heller, Jorge; Ng, Steven Y.
PA Advanced Polymer Systems, Inc., USA
SO U.S., 12 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5939453	A	19990817	US 1998-90648	19980604
	WO 9962983	A1	19991209	WO 1999-US11952	19990528
	W: AE, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, CZ, DE, DE, DK, DK, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9942204	A1	19991220	AU 1999-42204	19990528
	EP 1084170	A1	20010321	EP 1999-926034	19990528
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002517535	T2	20020618	JP 2000-552189	19990528
PRAI	US 1998-90648	A	19980604		
	WO 1999-US11952	W	19990528		

AB The title block polymers have both **hydrophilic** and **hydrophobic** blocks. They form micelles in an aq. soln., making them suitable for encapsulation or solubilization of **hydrophobic** or water-insol. materials. They also form bioerodible matrixes for the sustained release of active agents, esp. when the polyortho ester blocks contain at least one unit contg. an .alpha.-hydroxy acid. 3,9-Di(ethylidene)-2,4,8,10-tetraoxaspiro[5.5]undecane-PEG Me ether-cyclohexanedimethanol block copolymer 100 mg was dissolved in 2 mL acetone, and the soln. added to a soln. of 7.7 mg hydrocortisone in 2 mL acetone. The combined acetone solns. were added to 5 mL phosphate-buffered saline, pH 7.4, the acetone removed under vacuum, and the aq. soln. filtered through a 0.45 mm filter. The aq. soln. was found to have a hydrocortisone concn. of 1.1 mg/mL, approx. four times greater than the water soly. of hydrocortisone of 0.28 mg/mL, indicating micellar encapsulation and solubilization of the hydrocortisone by the copolymer.
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d kwic 5

L14 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2002 ACS
TI PEG-poly(**ortho ester**), PEG-poly(**ortho ester**)-PEG, and poly(**ortho ester**)-PEG-poly(**ortho ester**) block copolymers

AB The title block polymers have both **hydrophilic** and **hydrophobic** blocks. They form micelles in an aq. soln., making them suitable for encapsulation or solubilization of **hydrophobic** or water-insol. materials. They also form bioerodible matrixes for the sustained release of active agents, esp. when the polyortho ester. . .

IT Polyoxyalkylenes, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(block; spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

IT Antitumor agents
Micellization
(spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

IT 78-19-3, 3,9-Divinyl-2,4,8,10-tetraoxa-spiro[5.5]undecane 107-15-3, 1,2-Ethanediamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

IT 65967-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

IT 237739-72-9P 237739-73-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

IT 50-23-7, Hydrocortisone
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(spiroether group-contg. polyoxyalkylene polyether blocks for solubilization of **hydrophobic** agents)

(1967). Isoln and structure of *Nα-formyl melittin:* Lübke *et al., Experientia* **27,** 765 (1971). Synthesis of melittin and related peptides: Lübke, Schröder, *Peptides,* H. C. Beyerman, A. van der Linde, W. M. van den Brink, Eds. (North-Holland Publishing Company, Amsterdam, 1967) pp 271-279; Dorman, Markley, *J. Med. Chem.* **14,** 5 (1970); Schröder *et al., Experientia* **27,** 764 (1971). Synthetic congeners *melittin II* and *Nα-formyl melittin II* have been studied, *see* Schröder *et al., loc. cit.* Review of biochemistry and pharmacology: Habermann, *Science* **177,** 314 (1972).

Gly-Ile-Gly-Ala-Val-Leu-Lys-Val-Leu-Thr-Thr-Gly-Leu-Pro-
1 7 14

Ala-Leu-Ile-Ser-Trp-Ile-Lys-Arg-Lys-Arg-Gln-Gln-NH_2
15 26

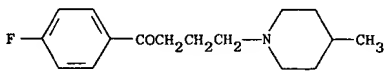
Cream white, water soluble powder. $[\alpha]_D^{21}$ −89.52° (c = 0.409).

THERAP CAT: Antirheumatic.

5644. Mellitic Acid. *Benzenehexacarboxylic acid;* mellic acid. $C_{12}H_6O_{12}$; mol wt 342.17. C 42.12%, H 1.77%, O 56.11%. $C_6(COOH)_6$. Preparation from carbonaceous material: Kiebler, U.S. pat. **2,461,749** (1949 to Carnegie Inst. of Tech.); Germain *et al., Bull. Soc. Chim. France* **1962,** 779; from tetrahalophthalic acid: Brusset, Uny, *ibid.* **1951,** 565; Juettner, U.S. pat. **3,067,246** (1962).

Crystals. mp 286-288° in sealed tube with decompn. Freely sol in water or alcohol; sol in boiling concd H_2SO_4 without decompn.

5645. Melperone. *1-(4-Fluorophenyl)-4-(4-methyl-1-piperidinyl)-1-butanone; 4'-fluoro-4-(4-methylpiperidino)-butyrophenone;* γ-(4-methylpiperidino)-*p*-fluorobutyrophenone; methylperone; flubuperone. $C_{16}H_{22}FNO$; mol wt 263.37. C 72.97%, H 8.42%, F 7.21%, N 5.32%, O 6.08%. Neuroleptic agent related structurally to haloperidol, *q.v.* Prepn: Belg. pat. **651,144** (1964 to Ferrosan), *C.A.* **63,** 13224c (1965). Distribution of ^{14}C melperone: N. Einer-Jensen, E. Hansson, *Acta Pharmacol. Toxicol.* **23,** 65 (1965). Pharmacological and toxicological studies: J. A. Christensen *et al., ibid.* 109; R. Heywood, A. K. Palmer, *Farmaco Ed. Prat.* **29,** 586 (1974). Dopamine-receptor binding in relation to clinical effect: I. Creese *et al., Science* **192,** 481 (1976). Sedative and sleep-inducing properties: R. Kretzschmer *et al., Arzneimittel-Forsch.* **26,** 1073 (1976). Clinical studies in anxiety: W. J. Poeldinger, *Therapiewoche* **30,** 4862 (1980); L. F. Fabre, M. J. Napoliello, *Curr. Ther. Res.* **30,** 427 (1981). Melperone has also been shown to have anti-arrhythmic effects: E. S. Platou *et al., Acta Pharmacol. Toxiol.* **50,** 108 (1982).

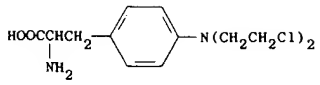


Liquid, $bp_{0.1}$ 120-125°.

Hydrochloride, $C_{16}H_{23}ClFNO$, *FG 5111, Buronil, Eunerpan.* Cryst, mp 209-211°. LD_{50} in rats, mice (mg/kg): 330, 230 orally; 40, 35 i.v., J. A. Christensen *et al., loc. cit.*

THERAP CAT: Neuroleptic.

5646. Melphalan. *4-[Bis(2-chloroethyl)amino]-*L*-phenylalanine; p*-di(2-chloroethyl)amino-L-phenylalanine; L-phenylalanine mustard; alanine nitrogen mustard; L-PAM; melfalan; L-sarcolysine; NSC-8806; CB 3025; Alkeran; Sarcoclorin. $C_{13}H_{18}Cl_2N_2O_2$; mol wt 305.20. C 51.16%, H 5.94%, Cl 23.23%, N 9.18%, O 10.48%. Syntheses: Bergel, Stock, *J. Chem. Soc.* **1954,** 2409; **1955,** 1223; *eidem,* U.S. pats. **3,032,584-5** (both 1962 to NRDC); Larionov, *Lancet* **2,** 169 (1955). Neurotoxicity study: M. G. Donelli *et al., J. Pharm. Pharmacol.* **18,** 760 (1966). Mutation study: J. McCann *et al., Proc. Nat. Acad. Sci. USA* **72,** 5135 (1975). Biliary excretion in rats: K. H. Byington *et al., Biochem. Pharmacol.* **29,** 2518 (1980). Review of carcinogenicity studies: *IARC Monographs* **9,** 167-180 (1975). *Review:* R. L. Furner, R. K. Brown, *Cancer Treat. Rep.* **64,** 559-574 (1980).



Needles from methanol (monosolvate), mp 182-183° (dec). $[\alpha]_D^{25}$ +7.5° (c = 1.33 in 1.0*N* HCl); $[\alpha]_D^{22}$ −31.5° (c = 0.67 in methanol). Soluble in ethanol, propylene glycol. Practically insol in water. LD_{50} in rats: 14.7 μmol/kg i.p., W. C. J. Ross, *Biochem. Pharmacol.* **13,** 969 (1964).

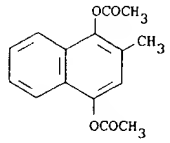
D-Form, *CB 3026, NSC-35051,* D-*sarcolysine, medphalan.* Needles from methanol (monosolvate), mp 181.5-182° (dec). $[\alpha]_D^{21}$ −7.5° (c = 1.26 in 1.0*N* HCl).

DL-Form, *merphalan, sarcolysine.* Tiny needles from methanol, mp 180-181°.

Human Toxicity: Bone marrow depression may occur. This substance has been listed as a carcinogen by the EPA: *Second Annual Report on Carcinogens* (NTP 81-43, Dec. 1981) pp 155-156.

THERAP CAT: Antineoplastic.

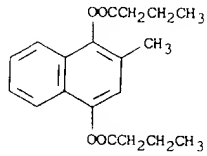
5647. Menadiol Diacetate. *2-Methyl-1,4-naphthalenediol diacetate;* acetomenaphthone; 2-methyl-1,4-naphthohydroquinone diacetate; 1,4-diacetoxy-2-methylnaphthalene; vitamin K_4; Kapilin; Kapilon; Prokayvit Oral; Vitavel K; Davitamon-K; Kappaxan; Kayvite. $C_{15}H_{14}O_4$; mol wt 258.26. C 69.76%, H 5.46%, O 24.78%. Prepd from naphthalene: Sah *et al., Ber.* **73,** 762 (1940); *Rec. Trav. Chim.* **59,** 461 (1940); by reductive acetylation of menadione: Horii *et al., Pharm. Bull. (Tokyo)* **5,** 82 (1957).



Crystals, mp 112-114°. Almost insol in water; slightly sol in cold alc; sol in 3.3 parts boiling alc, in acetic acid.

THERAP CAT: Prothrombogenic vitamin.

5648. Menadiol Dibutyrate. *2-Methyl-1,4-naphthalenediol dibutyrate;* 2-methyl-1,4-naphthohydroquinone dibutyrate; Karanum. $C_{19}H_{22}O_4$; mol wt 314.37. C 72.59%, H 7.05%, O 20.36%. Prepn: von Werder, Ger. pat. **734,220** (1943 to E. Merck).



Crystals, mp about 53°. Practically insol in water; sol in alcohol, benzene, oils and fats.

THERAP CAT: Prothrombogenic vitamin.

5649. Menadiol Diphosphate (Tetrasodium Salt). *2-Methyl-1,4-naphthalenediol diphosphoric acid ester tetrasodium salt;* 2-methyl-1,4-naphthohydroquinone diphosphoric acid ester tetrasodium salt; tetrasodium 2-methyl-1,4-naphthohydroquinone diphosphoric acid ester; menadiol sodium diphosphate; menadiol tetrasodium diphosphate; menadione diphosphate tetrasodium salt; Kappadione; Kipca, Water Soluble; Procoagulo; Synka-Vit; Synkayvite. $C_{11}H_8Na_4O_8P_2$; mol wt 422.09. C 31.30%, H 1.91%, Na 21.79%, O 30.32%, P 14.68%. Prepn from hydroquinone + phosphorus oxychloride: Fieser, Fry, *J. Am. Chem. Soc.* **62,** 228 (1940); from 2-methyl-1,4-naphthohydroquinone + phosphorus oxychloride: Kudryashov *et al., Voprosy Med. Khim.* **5,** No. 4, 279 (1959), *C.A.* **55,** 9517g (1961).